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Heirs of the revolution:

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X-ray diffraction and the birth of the

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Mineralogical Society of America

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Dedicated to J Alexander Speer on his retirement as Executive Director of MSA

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in thanks for his many years of selfless service

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Keywords: Mineralogical Society of America; Mineralogy; Crystallography;

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X-ray diffraction; History of Science

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ABSTRACT

25 The founding of the Mineralogical Society of America (MSA) in 1919 followed
26 so closely on the heels of the discovery of X-ray diffraction (XRD) in 1912 that one
27 might hypothesize a causal link. Was MSA born out of this scientific revolution? The
28 formation of our Society conventionally is attributed to the desire for a professional
29 journal and the need to emerge from the shadow of the Geological Society of
30 America, but these issues were not new in 1919. This review argues that MSA's
31 birth can be understood by an exploration of two historical strains: 1) Although
32 modern notions of atomism traditionally are associated with the emergence of the
33 kinetic theory of gases in the late 19th century, mineralogists had invoked ordered
34 atomic spheres as the fundamental metaphor for crystalline structures over a
35 century earlier, leading directly to WL Bragg's discovery of the atomic design in
36 halite; and 2) In contrast to the broader chemistry community, mineralogists were
37 uniquely poised to embrace X-ray diffraction and the revolution in crystallography
38 that attended it. This revelation gave rise to a sense of distinct identity.

39 An examination of MSA's early records unambiguously reveals that US
40 mineralogists were closely attuned to the crystallographic insurgency as it took
41 place across the Atlantic. In particular, Edgar T. Wherry, one of the organizers of the
42 *American Mineralogist* and of the Society, actively disseminated information about
43 the new discoveries to his colleagues in the United States. Other founders of MSA
44 similarly championed the insurgent character of the new crystallography, and they
45 argued that the discoveries differentiated mineralogy from other styles of geological
46 investigation, thereby warranting the establishment of a specialized professional

47 society. The continuing force of the revolution is revealed in a counter-reaction a
48 century later, as mineralogists have renewed their focus on phases at the boundary
49 between crystals and glasses, leading to reconsiderations of the meaning of
50 crystallinity.

51

52

INTRODUCTION

53 The six founders of the Mineralogical Society of America were born into a
54 world without atoms (Fig. 1). In December 1919, when MSA held its first meeting,
55 they ranged in age from 34 years (Edgar T. Wherry) to 53 (Alexander H. Phillips).
56 Thus, they all had received their scientific training in the classical 19th-century sub-
57 disciplines of mineralogy: Geometric Crystallography; Physical and Chemical
58 Properties of Minerals; Mineral Classification; and Descriptive Mineralogy. During
59 the 1890s, when most of the founders were working towards their graduate
60 degrees, the ultimate structure of crystalline materials was highly controversial, and
61 most mineralogy textbooks of the time adopted a wait-and-see agnosticism
62 concerning the physical reality of atoms.

63 Emblematic of the shift of US mineralogy away from European dominance,
64 half the founders received formal instruction in Europe and half learned their
65 mineralogy domestically. Edward H. Kraus, the first president and principal
66 architect of MSA, studied for his Ph.D. with Paul Groth in Munich from 1899 to 1901,
67 eventually assuming a mineralogy professorship at the University of Michigan (Hunt
68 1955). Frank R. Van Horn pursued a Ph.D. at the University of Heidelberg with
69 Victor Goldschmidt¹ from 1893 to 1897 and then became a professor at the Case
70 School of Applied Science (Kraus 1934). The Canadian Thomas L. Walker received
71 his Ph.D. in 1896 from the mineralogist Ferdinand Zirkel at the University of Leipzig,

¹ More specifically, Victor Mordechai Goldschmidt (1853-1933), who specialized in morphological crystallography and is distinguished from Victor Moritz Goldschmidt (1888-1947), who is considered the father of modern geochemistry.

72 and he then crossed paths with Van Horn as a postdoctoral associate with
73 Goldschmidt in Heidelberg (Parsons 1943).

74 The three remaining MSA founders were schooled primarily in the United
75 States. Alexander Phillips, born in next-door Lawrenceville, New Jersey, was a
76 Princetonian from his undergraduate A.B. to his graduate Sc.D. degree to his 49
77 years of college instruction at his alma mater (Buddington 1937). Herbert Whitlock,
78 curator at the American Museum of Natural History, studied with the famed
79 mineralogist Alfred Moses at Columbia University but prided himself on achieving
80 what he did without a doctorate (Pough 1949). The polymath Edgar Wherry
81 received his Ph.D. with Amos Peaslee Brown at the University of Pennsylvania in
82 1909, but he did spend one summer, in 1910, under the tutorship of Victor
83 Goldschmidt to deepen his knowledge of morphological crystallography (Hooker
84 and Montgomery 1975).

85 To the degree that six middle-aged, white American men of European
86 descent with a shared love of minerals can be considered eclectic, the founders
87 brought a mix of expertise to the table in 1919. In addition to his duties as
88 mineralogist, Van Horn acted as the athletic director at Case from 1900 to 1926, and
89 he oversaw the development of a high-level football program that toppled Ohio
90 State and Purdue (Grabowski 1992). Alexander Phillips's administrative skills as
91 chair of the organizing committee for MSA in 1919 were enriched by his tenure as
92 mayor of Princeton Township from 1911 to 1916 (Buddington 1937). Before
93 assuming his posts as professor at the University of Toronto and the first director of
94 the Royal Ontario Museum of Mineralogy, TL Walker was the assistant

95 superintendent of the Geological Survey of India from 1897 to 1901. His duties
96 included an arduous scientific expedition through the Himalayan Mountains from
97 India into Tibet. As a youth, ET Wherry collected plants before he discovered
98 minerals, and by the time he helped found MSA, he was working in the US
99 Department of Agriculture, eventually becoming a professor of botany at the
100 University of Pennsylvania in 1930.

101 Despite their different educational backgrounds and life experiences, as
102 American mineralogists advocating for the establishment of a new professional
103 society in 1919, these men were bound by a transformation within the previous
104 decade that had dramatically redrawn their intellectual landscapes. Whereas
105 nobody knew the fundamental structure of a mineral before 1912, by the end of that
106 decade, researchers across the Atlantic had established the paradigms for
107 crystallinity that still are taught in introductory mineralogy classes today.

108 To what extent was the founding of the Mineralogical Society of America a
109 response to the X-ray diffraction revolution? How did American mineralogists
110 perceive the relationship between atomic theory and crystallinity before the
111 revolution? Were they aware of the upheaval in European physics as they worked
112 to create MSA in the decade before its birth, and did they anticipate the vast impact
113 those discoveries would exert on the mineral sciences? How has the response of the
114 US mineralogical community to the XRD revolution evolved over the last century?
115 The synchronicity between the establishment of MSA and the transformation of
116 solid-state physics reasonably suggests some kind of linkage. On the other hand,
117 temporal correlation does not necessarily imply causation.

118 This celebratory article for the centennial anniversary of MSA explores the
119 intellectual framework that guided the six founders and their colleagues in the
120 invention of MSA. For the Society's fiftieth anniversary, George Phair of the United
121 States Geological Survey authored articles on the birth of *The American Mineralogist*
122 in 1916 and the society itself in 1919 (Phair 1969a,b). Whereas Phair skillfully
123 describes *how* MSA came into being, one can question whether he adequately
124 captures *why* the Society and its journal succeeded when prior efforts had failed.
125 Phair repeats the founders' argument that professional mineralogists desired a
126 dedicated periodical amidst a growing incompatibility with the Geological Society of
127 America (GSA), founded in 1888.

128 As will be argued below, this rationale must represent only a partial
129 explanation. The *American Journal of Science (AJS)* had served as an engine for
130 mineralogical research since its inception by Benjamin Silliman in 1818; in 1916
131 alone, 22 articles of a strictly mineralogical nature appeared in *AJS*. On the other
132 hand, several efforts to jumpstart purely mineralogical journals came to naught in
133 the late 19th and early 20th centuries. Thus, before 1916, mineralogists could not
134 sustain a journal of their own, but they could access a magazine that was prestigious
135 and communal with other branches of geology. From 1916 onwards, *The American*
136 *Mineralogist* inaugurated a journey that continues today under the auspices of a
137 thriving professional society founded three years later.

138 Something changed during that decade. Whereas MSA lore paints the
139 founders as reluctant exiles from an insufficiently convivial coalition of geologists,
140 this article asserts that MSA emerged as a separatist movement grounded in a new

141 sense of self-identity. Their feeling of distinctness originated in the redefinition of
142 minerals after the X-ray diffraction revolution. This interpretation will be assessed
143 through two theses: 1) MSA's founders descended from a long lineage in
144 mineralogical philosophy that nurtured notions of atomicity – specifically, of
145 crystals as ordered assemblages of hard spheres. Consequently, mineralogists were
146 primed to accept the implications of X-ray crystallography in the face of persistent
147 skepticism from gas and solution chemists; and 2) The empirical justification of the
148 metaphors that mineralogists used to describe crystalline materials provided the
149 impetus for US mineralogists to distinguish themselves from other kinds of Earth
150 scientists and create a scientific society that has flourished for 100 years.

151

152 **BEFORE THE REVOLUTION: MINERALOGISTS AND OUR CONCEPTIONS OF ATOMS**

153

154 **Unit Cells and Atomic Spheres**

155 In a retrospective of the X-ray diffraction revolution, Max Perutz, student of
156 William Lawrence Bragg and winner of the Nobel Prize for solving the structures of
157 hemoglobin and myoglobin, reviewed his mentor's accomplishments in the light of
158 Thomas Kuhn's theories of scientific revolutions (Perutz 1990; Kuhn 1996). He
159 asserts that "the perusal of old textbooks of chemistry and mineralogy has
160 convinced me that there was no paradigm for the atomic structure of solid matter
161 before 1912. The results of X-ray analysis opened a new world that had not even
162 been imagined before."

163 It is a significant overstatement, as Perutz failed to recognize that WL Bragg –
164 for all his undoubted genius – was the direct beneficiary of over a century of
165 mineralogical forays into the ultimate structure of crystals. Intimations of the
166 repetitive unit cells that embody the translational symmetry inherent to all crystals
167 are found in the geometrical crystallography of the French abbé and mineralogist,
168 Renée-Juste Haüy, who argued that mineral cleavage is controlled by *molécules*
169 *intégrant*es that act as the fundamental building blocks of crystals (Fig. 2). Haüy
170 (1784; 1801) posited an extravagantly large variety of geometric forms for his
171 integrant molecules – including octahedra, tetrahedra, hexagonal prisms, rhombic
172 dodecahedra, and hexagonal bipyramids, but his disciples corrected and refined his
173 speculations (Kubbinga 2012). Over the mid-1800s, Christian Samuel Weiss, Moritz
174 L. Frankenheim and Johann F.C. Hessel in Germany, Auguste Bravais in France, and
175 Alex V. Gadolin in Russia developed our more modern conceptions of space lattices
176 generated by parallelepipeds with constrained morphological symmetries (Weiss
177 1814; Frankenheim 1826; Hessel 1830; Bravais 1851; Gadolin 1867).

178 Similarly, the notion that matter ultimately is constructed from the assembly
179 of spherical particles has a deep history in the mineral sciences (Lalena 2006).
180 Johannes Kepler is credited as the first Western natural philosopher to propose that
181 the dense packing of small spherical particles underlies the structure of snowflakes
182 (Fig. 3A; Kepler 1611; Lima-de-Faria 1990); he famously conjectured that the 26%
183 void space within a cubic closest-packed array is the lowest value possible for an
184 assemblage of spheres. (This conjecture was not mathematically verified until the
185 proof by Thomas Hales in 2005.) Robert Hooke (1665) argued in *Micrographia*

186 *Restaurata* that quartz crystals are composed of spheroids (Fig. 3B), and in his
187 *Traité de la Lumière* (1690), the wave mechanic Christian Huygens depicted a
188 rhombohedral cleavage fragment from calcite as constructed from packed spheres
189 (Fig. 3C). William Wollaston, the British natural philosopher who refined the
190 reflecting goniometer, revived these ideas in his Bakerian Lecture to the Royal
191 Society in 1813, noting that the tetrahedra, octahedra and cubes that composed
192 Haüy's *molécules intégrantes* in turn could be constructed from the packing of
193 smaller spheres (Fig. 4). To generate the rhombohedral distortions required for
194 carbonate minerals, Wollaston flattened his spheres into ellipsoids (Wollaston
195 1813).

196 Contemporaneously, John Dalton – the “Father of Atomic Theory” – adopted a
197 physical model for atoms in which a spherical hard nucleus was enveloped by
198 repelling shells of “caloric” – the term for a hypothetical fluid responsible for heat
199 flow in substances. It was a somatic model earlier promoted by the Irish chemist
200 Bryan Higgins (Grossman 2017), but Dalton (1808) was the first to place atomism
201 on a quantitative footing by weighing common compounds and measuring ratios of
202 elemental masses. Dalton's insights included a recognition that individual elements
203 contain atoms of uniform size and mass, and his analyses revealed that these
204 different elements combine in simple integral ratios to make compounds (Fig. 5).

205 This work was greatly extended by the Swedish chemist and mineralogist
206 Jöns Jacob Berzelius. Berzelius innovated analytical techniques in chemistry and
207 measured the weights of thousands of compounds in support of Dalton's ideas
208 (Melhado 1981; Melhado and Frdnsgmyr 2003). Berzelius developed the system by

209 which we notate elemental symbols, and he created the molecular formula: H₂O,
210 SiO₂, and CaCO₃, for example, though he used superscripts (H²O) rather than
211 subscripts; one finds this superscript notation persisting in late nineteenth-century
212 mineralogy texts (Dana and Brush 1869). Berzelius intuited that compounds are
213 unions of electropositive and electronegative elements, and he was first to propose
214 a mineral classification system that embraced this principle (Berzelius 1814, 1824;
215 Heaney 2016).

216

217 **The Message in Isomorphs, Polymorphs, and Pseudomorphs**

218 The chemical permutations of similarly shaped minerals provided further
219 support for theories of atomism (Geiger 2016). Wollaston used his state-of-the-art
220 reflecting goniometer to show that the rhombohedral angles for “carbonate of lime”
221 (calcite), “bitter-spar” (magnesite), and “iron-spar” (siderite) are within 2° of each
222 other (Wollaston 1812). Though he is rarely credited with the discovery of
223 isomorphism (Morrow 1969), Wollaston inferred the existence of solid solution
224 based on the mixing of atoms in this system:

225 “It is very evident, from the numerous analyses that have been made of iron-
226 spar by other chemists, how extremely variable they are in their
227 composition, and consequently how probable it is, that the greater part of
228 them are to be regarded as mixtures.”

229 And he predicted that the carbonate isomorphs should extend to an as-yet-unknown
230 manganese variety – rhodochrosite, christened by the German mineralogist Johann
231 Hausmann the following year (Hausmann 1813).

232 Comparisons of synthetic potassium phosphate and arsenate crystals led to a
233 more sophisticated treatment (and naming) of isomorphism by the mineralogical
234 chemist Eilhard Mitscherlich (1819; 1821), who also saw in isomorphism a
235 confirmation of Dalton's notions of atomism (Melhado 1980; Moore 1990).
236 Mitscherlich (1822) further discovered the converse property of polymorphism, and
237 parallel to Wollaston's (1813) thesis, he viewed polymorphism as evidence that
238 discrete particles can assemble in different ways to generate different structures.
239 Importantly, minerals that had the same chemical composition but different crystal
240 structures defied Haüy's conflation of the primary "chemical molecule" of a mineral
241 with its physical integrant molecule.

242 Another mineral "-morphism" – pseudomorphism – also seemed explicable
243 only through a corpuscular theory of matter. The replacement of one mineral by
244 another with the retention of the original habit was telling testimony that elements
245 were composed of small, discrete particles that could interchange within crystals. In
246 his survey of mineral pseudomorphs, Dana (1845) (who used "atom" and "molecule"
247 interchangeably as was the custom of the time) argues that

248 "There appears to be something in the chemical forces excited among the
249 molecules, by the process of solution, when very slow and gradual, which
250 leads the molecules of any body that may be passing at the time from a liquid
251 state, to take the place successively of each molecule that is removed; and
252 thus it is that the original form to the minutest stria, is so exactly assumed by
253 the substituting mineral."

254 Consequently, pseudomorphism – a phenomenon once viewed as compelling
255 evidence for alchemical transmutation – could now be explained by "the received
256 principles of chemical science" of the mid-nineteenth century (Dana 1845).

257 From the first (1837) to the fourth edition of the *System* (1854), Dana
258 devoted several pages to a consideration of the particles from which minerals are
259 constructed. In his treatment, he elected to “adopt, in part, Wollaston’s theory of
260 spherical and spheroidal molecules...[which] by their aggregations, must produce
261 the same forms as proceed from the aggregation of Abbé Hauy’s polyhedral
262 molecules” (Dana 1837, pp. 53). In that first edition of his *System of Mineralogy*,
263 James Dwight Dana (pp. 69) makes clear his expectation that mineralogists would
264 lead the way to an understanding of the ultimate nature of matter:

265 “[W]e may be encouraged to hope that ere long this entrance to one of the
266 innermost recesses of the works of nature will be thrown open, and that the
267 qualities of atoms, or molecules, their forms and peculiarities, will soon be
268 fully understood. Its connection with the science of chemistry, and other
269 physical sciences, render it deserving of very minute experimental research.”

270 Dana’s intuition regarding the integral role of mineralogy in solving the first crystal
271 structures would be realized through a quirky and largely self-taught genius,
272 William Barlow, an amateur geologist and President of the English Mineralogical
273 Society from 1915 to 1918 (Fig. 6).

274

275 **A Prototype for Ionic Solids: The Work of Barlow and Pope**

276 William Barlow’s income came through an inherited family business, and by
277 his early thirties he had no need of a formal profession, freeing him to muse on
278 problems of three-dimensional crystallography. His long-time collaborator Pope
279 (1935) remarks: “It was never easy to follow his train of thought because he
280 invented his own ways of attaining results; thus, he rarely used the classical

281 methods of spherical trigonometry in crystallographic calculations, but devised
282 special ones of his own for each case which arose.” Independent of the techniques
283 employed by mathematicians Arthur Moritz Schönflies and Evgraf Federov, Barlow
284 elucidated space group theory, though he received less credit at the time because he
285 published a few years after they did and his approaches were sometimes inscrutable
286 (Barlow 1894; Pope 1935; Senechal 1990).

287 While he was working through the 230 space groups, Barlow simultaneously
288 was pondering the question of how spherical atomic particles might arrange
289 themselves to generate crystals. In 1883 he proposed a variety of packing schemes
290 for spherical atoms, including body-centered cubes and cubic- and hexagonal-
291 closest packed arrays, supplementing his sketches with accurate wooden models of
292 his own crafting (Fig. 7; Gibson 1941). He erred in assuming that electropositive
293 and electronegative atoms would have the same radii, leading him to propose, for
294 example, that halite occurs with a cesium chloride structure. Nevertheless, this
295 early work was striking for its attempt to marry the physical behavior of a crystal
296 with its internal atomic structure. Barlow (1883) argues, for example, that quartz
297 “has the property of circular polarisation, from which it has been proved that its
298 molecules must have a *spiral* arrangement” that could be either right- or left-
299 handed. Further, he modeled calcite by considering its chemical composition in
300 conjunction with its uniaxial optical behavior.

301 Although Barlow’s (1883) stacking of like-sized atoms in repetitive unit cells
302 got many details of crystal structures wrong, in 1898 he extended his ideas to
303 consider mixtures of different-sized atoms and produced a visualization (Fig. 8) that

304 would accurately presage WL Bragg's structure solution for NaCl in 1913. The link
305 between Barlow's penetrating insight and Bragg's subsequent "discovery" was
306 William Jackson Pope (Barlow and Pope 1906, 1907). Pope was Professor of
307 Chemistry at the School of Technology in Manchester when their partnership
308 started, and following publication of his work with Barlow, he fortuitously was
309 appointed Professor of Chemistry at Cambridge in 1908, placing Pope in direct
310 contact with WL Bragg, who entered Trinity College, Cambridge in 1909 and was a
311 first-year research student at Cambridge in 1912. Barlow and Pope (1906),
312 borrowing from theories of "atomic dynamism" dating from Boscovich (1758),
313 assumed that crystals represent equilibrium assemblages of balanced forces, with
314 each spherical atom acting as a center of both attraction and repulsion, both
315 governed by an inverse distance law by analogy with gravity.

316 Barlow and Pope (1907) surmise that the native elements are structured by
317 simple cubic or hexagonal closest packings of equal spheres; the novel powder X-ray
318 diffraction work by the American A.W. Hull would confirm that many (but not all) of
319 their assigned structures were correct (Hull 1922). The closest-packed models for
320 alkali halides are less accurate and would have benefited from a knowledge of
321 Pauling's Rules, whose formulation was still two decades away (Pauling 1929). But
322 in his reminiscences, WL Bragg (1962) nevertheless credited Pope and Barlow for
323 directing his initial X-ray diffraction trials to halite and sylvite:

324 "[W]hen my first studies of Laue's diffraction patterns led me to postulate
325 that zinc sulphide was based on a face-centred cubic lattice, Pope saw in it a
326 justification of his theory and urged me to experiment with sodium chloride
327 and potassium chloride crystals which he got for me from Steeg and Reuter
328 [a crystal optics firm] in Germany."

329 Equally significant, Barlow and Pope (1906, 1907) would provide Bragg with an
330 atomic template for deconstructing his diffraction patterns. Bragg's deference to
331 these early crystal theorists permitted him to eschew the conventional wisdom
332 upheld by virtually every contemporary chemist – that the crystals of alkali halides
333 must reflect diatomic pairings of alkali metals with halogen elements. Instead,
334 Barlow and Pope set the stage for Bragg's bold decision to model the first crystal
335 structure solved – that of halite – as cubic closest packed layers of spherical ions
336 without a hint of molecularity.

337

338 **ATOMIC DOUBTS BEFORE THE REVOLUTION**

339

340 **A Periodic Table Without Atoms?**

341 Ironically, while wet chemical assays, blowpipe tests, and elemental
342 spectroscopy achieved high levels of rigor in the latter half of the nineteenth
343 century, many chemists retreated from a categorical acceptance of physical atomism
344 (Brock and Knight 1965). Mendeleev's conception of the Periodic Table provides an
345 example. A suite of scientists in the 1860s argued that elements could be tabulated
346 on the basis of atomic weight: John Newlands in England, Julius Lothar Meyer in
347 Germany, and most famously, Dmitri Mendeleev in Russia (Kean 2011). Mendeleev
348 (Fig. 8A) asserted that chemical behavior was modulated as elemental masses
349 increase, and, based on the cyclic reactivity of elemental series, the Periodic Table
350 was born. The regularity was sufficiently remarkable that Mendeleev famously left
351 vacancies where undiscovered elements should reside. Indeed, in his original table,

352 Mendeleev knew that he should leave *two* spaces between zinc and arsenic (van
353 Melsen 1960).

354 The Periodic Table did not prove atomism, but it was highly suggestive that
355 the elemental series was composed by sequential additions of discrete particles.
356 Nevertheless, unlike Julius Meyer (Kaji 2002), Mendeleev’s views of atomism were
357 complex and equivocal (Niaz et al. 2004; Gordin 2019). On the one hand, Mendeleev
358 (1879) writes, “By replacing the expression of *atomic weight* by that of *elementary*
359 *weight*, I think we should, in the case of elements, avoid the conception of atoms.”
360 Conversely, Mendeleev (1891) argues that “The law of combining weights is
361 formulated with great ease, and is an immediate consequence of the atomic theory.
362 Without it, it is even difficult to understand.” Nevertheless, Mendeleev persistently
363 rejected the notion that atoms themselves could be divisible, and he was a vocal
364 antagonist to JJ Thomson in his identification of electrons as sub-atomic particles
365 (Kargon 1965).

366 Mendeleev’s ambivalence was steeped in a Positivist philosophy that
367 demanded a strictly empirical approach towards the apprehension of natural
368 processes and prevailed for much of the nineteenth century (Niaz et al. 2004). The
369 German acoustical physicist Ernst Mach (Fig. 8B) famously expressed his skepticism
370 of atomic theory in the context of logical positivism by averring that scientists must
371 differentiate between reality and those metaphors that fruitfully predict what our
372 senses perceive (Mach 1883, translated in Mach 1919; Brush 1968):

373 “The atomic theory plays a part in physics similar to that of certain auxiliary
374 concepts in mathematics; it is a mathematical *model* for facilitating the
375 mental reproduction of facts. Although we represent vibrations by the

376 harmonic formula, ... no one will fancy that vibrations *in themselves* have
377 anything to do with the circular functions.”

378 Mach conceded that atomic theory had a provisional usefulness, but only as a
379 heuristic idea that would be discarded as soon as a better theory appeared
380 (Blackmore 1972), and Mach’s opposition to the atomic theory became a hallmark of
381 his epistemological purity (Pojman 2011): “If belief in the reality of atoms is so
382 important to you, I cut myself off from the physicist’s mode of thinking, I do not wish
383 to be a true physicist, I renounce all scientific respect – in short: I decline with
384 thanks the communion of the faithful.”

385 Mach was not alone in his skepticism at the turn from the 19th to the 20th
386 century. Whereas some thermodynamicists like Ludwig Boltzmann rooted their
387 interpretations of energy flow in statistical models that demanded the existence of
388 moving atomic particles (Lindley 2015), prominent contemporaries were skeptical,
389 including Lord Kelvin, Wilhelm Ostwald, Josiah Willard Gibbs, and Pierre Duhem
390 (Fleck 1963; Chalmers 2014). Beyond the absence of direct sensory confirmation
391 for the reality of atoms, these thermodynamicists perceived a continuity in energetic
392 processes that seemed incongruent with the actions of discrete corpuscles. They
393 also were challenged in developing mathematical formulations for energy fluxes in
394 systems of atoms separated by vacuum. Ostwald, as co-editor of the influential
395 *Zeitschrift für Physikalische Chemie* and author of a widely admired textbook on
396 physical chemistry, strongly influenced this anti-atomic school. In his 1904 Faraday
397 lecture to the Chemical Society of London, he argued (Ostwald 1904):

398 “It is possible to deduce from the principles of chemical dynamics all the
399 stoichiometrical laws: the law of constant proportions, the law of multiple

400 proportions and the law of combining weights... Chemical dynamics has,
401 therefore, made the atomic hypothesis unnecessary..."

402 Josiah Gibbs concurred in his introduction to *Statistical Mechanics* (Gibbs 1902):

403 "Certainly, one is building on an insecure foundation, who rests his work on
404 hypotheses concerning the constitution of matter," citing the lack of agreement
405 between theory and experiment for the number of degrees of freedom exhibited by
406 a diatomic gas molecule.

407

408 **The Structure of Matter in Mineralogy Texts**

409 Mineralogists of the time mirrored this unsettled state. Dana's *System*
410 retreated from its earlier progressive role in championing atomic theory and skirted
411 the subject in later editions. Whereas Dana's *System* promoted atomism from the
412 first (1837) to the fourth edition (1854), JD Dana omitted all discussion of the
413 ultimate constituency of matter in the fifth edition of the *System* (1869) and beyond.
414 Ironically, the fifth edition is considerably more explicit than the fourth in its
415 appropriation of atomic theory to describe mineral chemistry. It includes a table of
416 atomic weights in alphabetical order, and it discusses mineral formulas with respect
417 to atomic ratios and masses much more comprehensively than did prior editions.

418 As inorganic chemistry became rigorously quantitative in the second half of
419 the nineteenth century, JD Dana may have decided that conjectures concerning the
420 shapes and arrangements of atomic particles were too speculative and unscientific.
421 Richard Harrison Solly, the demonstrator in mineralogy at Cambridge, explicitly
422 expresses this sentiment in his manual (Solly 1894):

423 “There is still complete ignorance as to which of the possible geometrical
424 structures suggested by Bravais, Groth, Sohncke and Liveing, can and does
425 really exist. We can say that a system of atoms grouped in a certain manner,
426 will have certain symmetry but we do not know whether they can remain in
427 equilibrium and subsist. To solve this problem we must possess an increased
428 knowledge of molecular forces.”

429 In his influential mineralogy textbook, the German mineralogist Paul Groth (1906)
430 treats atoms as objects of theoretical utility. He approvingly cites Sohncke’s (1888)
431 interpretation of a crystal as “a finite number of interpenetrating regular point
432 systems, which all possess like and like-directed coincidence movements,” such that
433 each point “may equally well be supposed to be occupied by similar *atoms*, as by
434 *molecules*.”

435 Groth anticipates the lack of molecularity in ionic solids: “It is evident,
436 however, that in such a structure ‘molecules,’ in the sense in which we speak of
437 gaseous molecules, are altogether wanting, and it is a matter of choice what is to be
438 called the unit of crystal structure or the crystal molecule.” In parallel, many
439 mineralogy textbook writers wrestled with the question of whether chemical
440 formulas are imprinted somehow within a crystal structure. MSA founder
441 Alexander Phillips of Princeton, for example, asserts (Phillips 1912): “There is no
442 method of demonstrating whether the solid or crystalline molecule and the chemical
443 molecule are identical. Since a number of atoms combine to form a chemical unit, it
444 is also probable that a number of chemical units combine to form a crystalline unit
445 or molecule.”

446 In his mineralogy textbook, Henry Miers, mineralogy professor at Oxford and
447 Fellow of the Royal Society, described the same state of confusion. Interestingly,

448 Miers offers the following pragmatic assessment of crystals that escaped many of
449 the thermodynamicists of the time (Miers 1902):

450 “It is reasonable to suppose that the particles of which a crystal consists are
451 placed side by side in some regular arrangement, like the men in a battalion
452 of soldiers; whereas in an amorphous substance they have no regular order.
453 Without some such hypothesis it is impossible to understand how the
454 properties of a crystal vary regularly with the direction.”

455 It is important to note that Miers uses the term “particles” rather than “atoms” in
456 this context, because he liberally employs the word “atom” elsewhere when he is
457 dealing with chemical rather than physical units. Similar efforts to adopt atomic
458 theory but to elide any speculations regarding the physical nature of atoms also are
459 apparent in the pre-revolutionary mineralogy texts of Moses and Parsons (1900),
460 WS Bayley (1910), and ES Dana (1912).

461

462 **1909-1919: THE CRYSTAL REVOLUTION**

463

464 **The Atom as a Physical Entity**

465 The existence of atoms was resolved rapidly and decisively in the decade
466 before the birth of MSA. At the beginning of this decade, an image of the physical
467 structure of atoms was taking form through the cathode ray tube studies of JJ
468 Thomson, who developed a “plum pudding” model for the atom, in which negatively
469 charged electrons are embedded within a positively charged matrix, like raisins
470 within dough (Thomson 1904). In 1911, Ernst Rutherford dispensed with this
471 metaphor on the basis of his high-angle scattering experiments, arguing
472 persuasively that backscattering of α - and β -particles by gold foil could be explained

473 only by a concentration of positive charge in a small, central nucleus (Rutherford
474 1911).

475 The next year, 1912, the momentous X-ray diffraction experiments of Max
476 von Laue resulted in the integration of crystallinity with atomic theory. Max Laue
477 (Fig. 10), a Privatdozent in physics at the Ludwig Maximilian University of Munich,
478 was stimulated by a discussion of Paul Ewald's doctoral dissertation to consider the
479 scattering of X-ray radiation by an ordered lattice of polarizable atoms (Laue 1962).
480 With Arnold Sommerfeld's half-hearted permission, two assistants – Walther
481 Friedrich, who had finished a doctoral thesis with Röntgen and was serving as an
482 assistant to Sommerfeld, and Paul Knipping, a doctoral student with Sommerfeld –
483 were set to the task of demonstrating X-ray diffraction by a crystal of copper sulfate
484 (Friedrich et al. 1912; 1913). The revelations that we associate with this discovery
485 today were not instantly evident (Fig. 11). Laue originally hypothesized that
486 secondary fluorescent X-rays generated from *within* a crystal would diffract from
487 the crystalline lattice, so Friedrich initially placed photographic plates to the *sides* of
488 the copper sulfate crystal, and even *between* the incident X-ray beam and the crystal,
489 before actually observing scattered X-rays when a plate was placed *behind* the
490 crystal (Forman 1969; Eckert 2011). Equally misguided, William Henry Bragg
491 initially interpreted Laue's diffractions as a focusing of X-ray corpuscles along
492 “avenues” between the crystal's atoms (Bragg WH 1912).

493 WH Bragg's perspicacious son, William Lawrence Bragg, bested his father by
494 inferring a wave-like nature for X-rays from von Laue's data (Fig. 12A), and he
495 outdid von Laue by recognizing that white X-radiation was selectively reflected from

496 “sets of parallel planes on which the atom centres may be arranged” (Bragg WL
497 1912). He followed with a presentation to the Cambridge Philosophical Society
498 (November 1912) and paper (January 1913) that accounted for Laue’s diffraction of
499 zinblende (sphalerite) according to his famous law: $n\lambda = 2d \cos \theta$ (when θ is
500 measured from the normal to the plane, by analogy to Snell’s law) (Fig. 12B; Bragg
501 WL 1913a; Perutz 1990). Only 22 years old at the time, WL Bragg thereupon
502 published the first crystal structure, of the halite crystal loaned to him by Pope
503 (Bragg WL 1913b), and père et fils followed with the structure of diamond (Bragg
504 WH and Bragg WL 1913). Within another year, WL Bragg single-authored solutions
505 to the structures of fluorite, sphalerite, pyrite, calcite and dolomite (Bragg WL
506 1914).

507 At this same time, the nature of those atomic scatterers came into sharper
508 focus thanks to a lifelong friend of WL Bragg and a student of Rutherford, Niels Böhr
509 (Fig. 13). Rutherford was puzzled by his own model for the atom, because classical
510 mechanics predicted that negatively charged electrons orbiting a positively charged
511 nucleus would degenerate as the electrons lose energy and spin into the core. Niels
512 Böhr solved this paradox by unifying the quantum theory of Max Planck with
513 elemental emission spectra collected over the previous half century. He proposed
514 that electrons encircle the positively charged nucleus of the atom in inherently
515 stable, energetically quantized orbitals (Böhr 1913; Rhodes 1986). He mailed his
516 landmark paper to Rutherford in March 1913, and later that year received
517 additional experimental vindication from the X-ray scattering work of Henry
518 Moseley. Killed in World War I only 2 years later at the battle of Gallipoli, Moseley

519 systematically explored the relationship between the frequency of an element's
520 characteristic K_{α} X-ray and the nuclear charge of the element. His observation that
521 the frequency varies as the square of the charge provided a rigorous method for
522 identifying elements, and it quantitatively distinguished between atomic number
523 and atomic mass (Moseley 1913; Assmus 1995; Aulthier 2013).

524 The mathematical forms for describing diffraction came next (reviewed in
525 James et al. 1948). WL Bragg was more physicist than mineralogist, and to his later
526 chagrin he developed his own notation for the X-ray “reflecting planes” that
527 betrayed his ignorance of the Miller indices devised in 1825 by Cambridge
528 mineralogy professor William Whewell (Hunter 2004). The reciprocal nature
529 inherent in the Miller plane notation fortuitously presaged the inverse relationship
530 between real space and diffraction space. In 1912, Laue offered a “geometrical
531 theory” of the diffraction process that mathematically captured the scattering of X-
532 rays by a three-dimensional grating (Laue 1912). Paul Ewald (Fig. 14A), who
533 studied the scattering of visible light by periodic arrays of oscillating dipoles for his
534 Ph.D., quickly absorbed its implications and unified Laue’s physics with X-ray
535 diffraction phenomena to develop a new mathematical formalism: the reciprocal
536 lattice, such that $\vec{a} \cdot \vec{a}^* = 1$ where \vec{a}^* is normal to \vec{b} and \vec{c} , etc. Using this new
537 reciprocal space basis, he further expressed the conditions for diffraction through
538 the construction of the “Ausbreitungskugel”, literally, the “scattering sphere”, but
539 what we now call the “Ewald sphere” (Fig. 14B; Ewald 1913; Aulthier 2004).

540 Additional contributions to the interpretation of X-ray diffraction patterns
541 were immediately forthcoming (Buerger 1990). Laue was surprised that left- and

542 right-handed quartz crystals apparently gave rise to the same diffraction pattern,
543 and Georges Friedel explained this observation by noting that the diffraction
544 process inherently adds a center of symmetry, which today we know as Friedel's
545 law (Friedel 1913). Peter Debye, another Sommerfeld student, deduced a correction
546 for the decrease in X-ray diffraction intensity caused by thermal agitation of atoms
547 (Debye 1913), and CG Darwin, grandson of the famed evolutionary biologist,
548 developed additional correction factors for the effects of polarization and for
549 increasing diffraction order n , later to be known as the Lorentz correction factor
550 (Darwin 1914).

551 Two years later, in 1916, Peter Debye and Paul Scherrer developed a camera
552 specifically for diffraction from powders, a technique that would flourish among
553 Earth scientists for mineral identification (Debye and Scherrer 1916). Albert
554 Wallace Hull, the US physicist employed with General Electric, heard a guest lecture
555 by WH Bragg in 1915 and invented a different powder diffraction geometry that has
556 found renewed importance in the modern age of digital imaging plates (Hull 1917a).
557 Hull used it to determine the crystal structure of α -iron (Hull 1917b), which had
558 eluded the Braggs, and eventually published the structures of over 25 native
559 elements (Hull, 1922, 1946; Aulthier 2013).

560

561 **Ionic and covalent chemical bonding models appear**

562 The modern metaphors we use to understand the bonding of atoms in
563 crystals also emerged in the decade before MSA's founding. The chemical duality
564 implicit in our picture of crystals as marriages of electropositive and electronegative

565 elements appeared in the work of Berzelius and Faraday in the early 1800s
566 (Berzelius 1814; Melhado 1981). A century after Berzelius's ground-breaking work,
567 Erwin Madelung (1909) examined the energetic implications of crystals as arrays of
568 positively charged metal ions electrostatically attracted to negatively charged non-
569 metallic ions.² He intuited that attraction was limited by repulsions arising from
570 electronic shells surrounding atomic nuclei, and this model did remarkably well in
571 predicting the energies of formation for alkali halides (Wooster 1990).

572 In contrast to this model for an ionic solid, Gilbert Lewis – a professor of
573 chemistry at UC-Berkeley – realized that in nonpolar molecules the electrons
574 between atoms are shared rather than exchanged, and in 1916 he wrote the
575 template for covalent bonding (Lewis 1916), complete with the dot notation that we
576 still employ to describe valence electrons (Fig. 15). Lewis published major works in
577 many areas, coining the terms “fugacity” (Lewis 1908) and “photon” (Lewis 1926),
578 and he perhaps is most famous for his theory of acids and bases. In his prescient
579 1916 paper, Lewis interpreted covalent bonding as a mechanism to complete the
580 outer electron shell. Building on Lewis's work (and winning a Nobel prize instead of
581 Lewis), Irving Langmuir introduced the term “covalence” to describe the sharing of
582 electrons between atoms in the year of MSA's birth (Langmuir 1919).

583

² The word “ion” derives from the Greek for $\iota\omicron$, meaning “I go”, based on Faraday's observations of their migration toward electrically charged poles (Van Melsen 1960).

584 **VIEWING THE X-RAY REVOLUTION FROM THE OTHER SIDE OF THE ATLANTIC**

585

586 **Edgar Wherry: America's Evangelist for the XRD Revolution**

587 Thus, in the space of a single decade our modern understanding of crystal
588 chemistry was born. By 1919, minerals could be visualized as ordered arrays of
589 atoms with positively charged cores enveloped by quantized electron orbitals that
590 swap or share electrons to fill valence shells and lower the energy state of the
591 atomic collective. To assess whether the impact of this sweeping transformation
592 ignited the origin of MSA, one must answer two questions: What did American
593 mineralogists know about the XRD revolution, and when did they know it? If the
594 work of von Laue and the Braggs eluded the founding members, then demonstrating
595 a connection between the birth of MSA and the XRD revolution is short-circuited at
596 the outset.

597 But the evidence is clear that the founding members *did* know about the
598 exciting developments in Britain and Germany, and they recognized their relevance
599 to mineralogy, thanks largely to the efforts of founding member Edgar T. Wherry,
600 who served as an assistant professor of mineralogy at Lehigh University from 1908
601 to 1913 and then as an assistant curator of mineralogy at the Smithsonian
602 Institution until 1917 (Hooker and Montgomery 1975). Over his career, Wherry
603 was a prolific author of papers at the intersection of mineralogy and botany, and
604 arguably his most significant scientific contribution was the recognition that
605 bentonite clays are of an igneous rather than sedimentary origin (Wherry 1917a);
606 this insight kick-started the application of bentonite beds for precise stratigraphic

607 correlation, and it also has marked bentonites as records of global volcanic events
608 (Kolata et al. 1996; Christidis and Huff 2009).

609 In 1916, Wherry was recruited by 19-year-old Samuel Gordon, assistant
610 curator of the Academy of Natural Sciences in Philadelphia, and H.W. Trudell, a
611 member of the Philadelphia Mineralogical Society, to launch the *American*
612 *Mineralogist* (Fig. 16; Phair 1969a). W.G. Levison, secretary to the New York
613 Mineralogical Club, for a short time served as the inaugural Editor-in-Chief, but he
614 withdrew at the close of 1918 when it became clear that Wherry was running the
615 show. The first six issues that year (July through December) were devoted largely to
616 descriptive mineralogy. Wherry warned in a letter to Gordon that “Perhaps the
617 greater part of our readership will be amateurs..., and if we put in too much
618 unintelligible high-brow dope they will not renew their subscriptions.” (Quoted in
619 Phair 1969a)

620 Nevertheless, Wherry and his co-editors found ways to highlight discoveries
621 in X-ray diffraction. The first mention of the Braggs appears in the March 1917
622 edition of *American Mineralogist* through a review of Irving Langmuir’s paper on the
623 fundamental properties of solids (Wherry 1917b):

624 “The work of the Braggs and others on the study of crystal structure with the
625 X-ray is reviewed, and the structures are described which have been found to
626 exist in the minerals halite, sylvite, diamond, sphalerite, fluorite, pyrite,
627 hauerite, calcite, dolomite, rhodochrosite, siderite, magnetite, spinel, copper,
628 silver, gold, lead, sulfur, quartz, zircon, rutile, and cassiterite. The inevitable
629 conclusion is admitted – that in... these substances, which belong to the class
630 of ‘polar compounds,’ the whole crystal must be regarded as a single
631 molecule.”

632 The June 1918 volume was dedicated to the 175th anniversary of the birth of René
633 Juste Haüy, and with this issue “*The American Mineralogist* came of age,” in the
634 estimation of Phair (1969a), earning the journal international esteem and attracting
635 a spike in subscriptions and advertisements. The multi-lingual Wherry (1918)
636 summarized articles from German and even Japanese journals that otherwise were
637 inaccessible to the readership for his “Abstracts of the Crystallographic Literature,”
638 a section that highlighted 33 recent articles of mineralogical relevance. Twenty-one
639 of these explicitly dealt with the X-ray diffraction of crystals, and Wherry continued
640 abstracting XRD-based articles in multiple issues in 1919.

641 Moreover, Wherry proselytized for the new crystallography through lectures
642 to the major mineral clubs. In the “Notes and News” section of the May 1917 issue
643 of the *American Mineralogist*, Levison conveys the sophistication of Wherry’s
644 presentation to the New York Mineralogical Society (Levison 1917):

645 “Dr. Wherry's paper consisted of a historical sketch and detailed review of
646 the revelations resulting originally from the suggestion by Dr. Laue of Zurich,
647 of employing a crystal as a "space diffraction grating" for X-rays, the
648 successful realization of the idea by Messrs. Friedrich and Knipping in 1912,
649 and its subsequent more elaborate and effective development by Messrs.
650 W.H. and W.L. Bragg, whereby great progress has been attained on the one
651 hand in our knowledge of the nature of X-rays, and on the other of the
652 architecture of crystals, or the disposition within them of the various
653 elementary atoms of which they are constructed.

654 “Dr. Wherry’s review was illustrated with blackboard formulas, adjustable
655 models of the atomic structure of crystals, and a series of lantern slides
656 showing the X-Ray Spectrometer and the evidence it has afforded of crystal
657 structure by both the photographic and ionization methods, taken largely
658 from the recent treatise on the subject by W.H. and W.L. Bragg.”

659 In a following note, Samuel Gordon records that Wherry gave the same talk for the
660 Philadelphia Mineralogical Society (Gordon 1917); likely, he did so for other East
661 Coast mineralogy clubs as well.

662

663 **First Depictions of Crystal Structures in *The American Mineralogist***

664 Wherry's (1918) "Abstracts" include the first atomic drawings of mineral
665 structures published in *The American Mineralogist*. In a preface intended so that
666 "space-lattices may be intelligible" to the reader, Wherry himself illustrates five
667 structure types: 1) Double face-centered cubic or diamond; 2) Simple cubic; 3)
668 Body-centered cubic; 4) Face-centered cubic; and 5) Combinations of different
669 lattices (Fig. 17). To our modern eyes, these depictions err in basic ways. For
670 example, halite and galena are classified as simple cubes rather than as face-
671 centered cubes, and hexagonal symmetries have no representation.

672 In addition, the concept of a spherical atom had not survived the Atlantic
673 crossing intact. In Wherry's diagrams, "the heavy dots represent the *positions of*
674 *centers of gravity of atoms* [italics added]." The "shape of each atom," as drawn by
675 Wherry, belonged to one of several polyhedra, "which may perhaps be regarded as
676 the 'integral molecules' sought by Haüy." Indeed, whether the point scatterers
677 described by the Braggs represented individual atoms or molecular clusters was a
678 point of heated debate through the 1920s (Miers 1918; Rogers 1921; Armstrong
679 1927). In addition to perceptions that the Bragg structures violated contemporary
680 valence theory (Pfeiffer 1917; Smits and Scheffer 1917), scientists subscribed to
681 Newton's dictum that nature abhors a vacuum. Unlike spheres, polyhedra can fill all

682 available space when closest packed. Moreover, chemical reactions of the common
683 elements proceeded in such a way as to fill the outermost shells with 8 electrons. A
684 cube has 8 corners. Could that be coincidence? And so one finds that the US
685 chemists Gilbert Lewis (1916) and Irving Langmuir (1919) promote atoms with
686 “cubical” rather than spherical symmetry (Fig. 18). It is evident that Wherry
687 likewise had not yet absorbed Bragg’s reconciliation of Barlow and Pope’s closest-
688 packed atomic spheres with the translational symmetry of the Bravais lattices.

689 Although he was arguably its most ardent advocate, Wherry was not the only
690 American mineralogist who recognized the impact of the X-ray diffraction
691 revolution. In the fifth edition to their *Elements of Mineralogy, Crystallography, and*
692 *Blow-Pipe Analysis*, Moses and Parsons (1916) already were referencing the 1915
693 text by the Braggs on *X-rays and Crystal Structure*. E.H. Kraus, the first president of
694 MSA, saluted their achievements in the preface to his textbook *Mineralogy: An*
695 *Introduction to the Study of Minerals and Crystals* (Kraus and Hunt 1920):

696 “Many of the important laws in physics, especially those relating to the
697 properties of light, have been studied principally on crystallized minerals.
698 The Nobel prizes in physics for 1914 and 1915 were awarded to Laue and the
699 Braggs (father and son) for epoch-making investigations upon the structure
700 of crystallized minerals by means of the x-ray.”

701 Similarly, on the West Coast, Austin Flint Rogers, professor of mineralogy at
702 Stanford, concludes in his *Introduction to the Study of Minerals and Rocks* (1921)
703 that

704 “The X-ray analysis of crystals combined with a mathematical study of the
705 possible arrangements of points in space has furnished us with a means of
706 determining the stereochemistry of the solid or crystalline state and has thus
707 thrown new light on the structure of matter. This work also promises to be of

708 value in settling many doubtful questions concerning crystals. It has truly
709 opened up one of the most interesting fields in the whole realm of science.”

710 Rogers also offers the most sophisticated discussion of space groups and X-ray
711 diffraction in a mineralogy text to that date, devoting 13 pages (pp. 133-146) to the
712 topic.

713

714 **DID MSA NEED THE XRD REVOLUTION TO INVENT ITSELF?**

715 The historical record reveals without ambiguity that the founding members
716 of MSA were aware of the import of X-ray diffraction to the mineral sciences before
717 the society was founded. Would they have created MSA in 1919 had von Laue and
718 the Braggs conducted their experiments a decade later? The evidence for a cause-
719 and-effect relationship between the XRD revolution and the birth of MSA is real but
720 indirect. Naysayers might cite two arguments to dissociate these events:

721 1) Contemporary accounts of the motivation for forming MSA placed strongest
722 emphasis on the need for a specialized journal; and 2) MSA was following rather
723 than leading international trends in the professionalization of mineralogy. Of
724 greater significance, however, are two supporting arguments: 1) As illustrated in
725 the preceding discussion, mineralogists were even better prepared than many
726 chemists to accept the lack of molecularity inherent in the Bragg model for ionic
727 crystals; and 2) As will be explored in the next sections, the XRD revolution offered a
728 redefinition of mineralogy that encouraged a new sense of separateness from
729 geologists.

730

731 **A Need to Detach from GSA**

732 At the end of his term as the inaugural president of MSA in 1920, University
733 of Michigan mineralogist Edward Kraus offered a review of the long- and short-
734 range factors that led to MSA's formation. Of the latter, he points to a recent
735 specialization in US mineralogy that could no longer be accommodated by the
736 Geological Society of America. The first two decades of the twentieth century was a
737 time of enormous investment in domestic science and in higher education, and
738 mineralogy was a major beneficiary (Kraus 1921):

739 “During this period, the development of science was indeed marvelous. This
740 statement applies to no science more than it does to mineralogy, by which
741 term we obviously include what may be readily interpreted as the broader
742 field, namely crystallography. Moreover, it was during the war that the
743 prominent position of the United States in the production of minerals and
744 mineral products, and the vastness of our mineral resources, were brought
745 most forcibly to the attention of the general public.”

746 As increasing numbers of scientists self-identified as mineralogists, they found GSA
747 conferences less congenial and editors of GSA journals less receptive to their
748 articles. Kraus (1921) notes that mineralogists “soon felt that aside from the social
749 aspect of the meetings, the society offered them but little in their own field.”

750 An attempt to form MSA was essayed in 1913. Alexander Winchell³,
751 professor of mineralogy at the University of Wisconsin, circulated a letter in January
752 of that year among ~20 mineralogists to address the possibility of organizing the
753 “National Association of Mineralogists and Petrologists.” The response to the

³ Alexander Newton Winchell (1874-1958) is not to be confused with Alexander Winchell (1824-1891), a co-founder of GSA and a controversial professor of geology and paleontology at the University of Michigan for his racist attitudes towards evolution

754 proposed separation from GSA was lukewarm, telling evidence that the mineralogy
755 community at this late date still was unprepared to stand on its own. Instead, the
756 community decided to explore an alternative to divorce. In an effort at
757 accommodation, GSA offered to provide sectional mineralogy-based meetings, but
758 over the next three years they never materialized (Phair 1969b).

759 The true seeds of change began with a meeting of the six founders in
760 December 1916 at the annual GSA conference in Albany, New York to discuss the
761 establishment of a new mineralogical society. Winchell eventually would serve as
762 president of MSA in 1932, but he was not a part of this renewed effort. Instead,
763 Messrs. Kraus, Phillips, Van Horn, Walker, Wherry, and Whitlock circulated a letter
764 (Fig. 19) in 1917 to 51 mineralogists in the US and Canada to argue that “the
765 founding of a Mineralogical Society would do much to stimulate greater interest in
766 the subject and also give wider recognition to the work being done in this field in
767 America.” Consequently, “the time has come when an organization which might be
768 called ‘The Mineralogical Society of America’ should be formed at as early a date as
769 possible.”

770 This exploratory letter emphasizes the need for a specialized journal as the
771 primary driving force for establishing MSA (Phair 1969b):

772 “[P]erhaps the greatest benefit to be derived would be the founding by the
773 society of a journal to be devoted exclusively to the publishing of
774 mineralogical papers. As is well known, there is great need for a dignified
775 medium of publication for the increasing volume of mineralogical
776 investigations which are being carried on in America.”

777 It was not a new complaint. Mineralogy journals had come and gone in the United
778 States for over a century. In fact, *The American Mineralogical Journal*, started by
779 New York City physician Archibald Bruce (who identified the eponymous Mg
780 hydroxide mineral), was “the first specialized American scientific periodical”,
781 running from 1810 to 1814 (Bruce 1968; Greene and Burke, 1978).

782 In his presidential address, Kraus (1921) provides a detailed overview of the
783 rise and fall of American mineral societies and the often transient journals that
784 attended their limited existence. Typically, these magazines were published by
785 mineral enthusiasts with careers outside the field, and their journalistic
786 experiments ended when the individuals fell ill, passed away, or found themselves in
787 financial embarrassment. In this regard, the long-lived success of Benjamin
788 Silliman’s *American Journal of Science* was truly an aberration (Brown 2014). The
789 Yale mineralogist founded *AJS* in 1818, and *AJS* is the oldest continually published
790 scientific journal in the US. Even in 1916, *AJS* was receptive to articles that were
791 narrowly mineralogical. One finds papers on the variable compositions and optical
792 behaviors of natural melanochalcite (Hunt and Kraus 1916), bornite (Allen 1916),
793 and hydro-zincite (Ford and Bradley 1916b), as well as reports of new minerals and
794 crystal growth processes (Phillips 1916; Ford and Bradley 1916a; Taber 1916).
795 Indeed, some of the first X-ray crystallography papers on minerals published by an
796 American scientist appeared in *AJS* rather than the *American Mineralogist* (e.g.,
797 Wyckoff 1920; 1921; 1925). On the other hand, entire monthly issues sometimes
798 were bereft of mineralogy, devoting space instead to articles on paleontology,
799 sedimentology, volcanology, atmospheric sciences, and experimental chemistry.

800 Of pressing concern to the founders, efforts to establish strictly mineralogical
801 magazines repeatedly sputtered. *The Young Mineralogist and Antiquarian* (1994-
802 1885) yielded to the *Mineralogists' Monthly* (1885-1892), which joined forces with
803 *Goldthwaite's Minerals* (1892-1894) to be reborn as *The Mineral Collector*, which
804 ceased publication in March 1909. The *Collector* had successfully straddled the
805 amateur and professional communities for 15 years, but its publisher, Arthur
806 Chamberlain, a printer, discontinued it for health reasons. The very first article in
807 the first issue of *American Mineralogist* pays tribute to Chamberlain's efforts (Bates
808 1916). Moreover, with the onset of World War I, German outlets such as *Zeitschrift*
809 *für Kristallographie, Mineralogie und Petrographie* interrupted publication for many
810 years and were anyway unreceptive to American contributors.

811 It was the death of *The Mineral Collector* that drove Samuel Gordon, assistant
812 curator at the Academy of Natural Sciences in Philadelphia, to initiate a new journal
813 with support from the Philadelphia Mineralogical Society, the New York
814 Mineralogical Club, and the now-defunct Mineral Collector's Association (Phair
815 1969a). Gordon had no academic degrees in mineralogy but received training
816 through Edgar Wherry, and Phair (1969a) identifies Gordon rather than Wherry as
817 the guiding force in putting together a staff and, against considerable financial and
818 logistical odds, creating the *American Mineralogist* (or more precisely, *The American*
819 *Mineralogist* since the definite article was dropped from the masthead only in 1988).
820 Wherry was trusted and respected by both the academic and amateur communities,
821 and Gordon enlisted Wherry to bridge these not always compatible populations.

822 As Kraus and colleagues looked to build a professional society, their respect
823 for the fledgling journal suggested that, given the costs and the challenges in
824 recruiting a subscriber base, adopting *The American Mineralogist* made more sense
825 than developing a competing journal. The staff of the magazine were receptive, and
826 Whitlock (1920) announced in a message to *Science* the intent to “enlarge the
827 *American Mineralogist* to include research papers and abstracts, but at the same
828 time to retain the valuable features of this publication which has become recognized
829 as of permanent interest to such collectors and amateurs who are eligible for
830 membership but not fellowship.” “Fellows,” in this prospectus for MSA, were
831 differentiated from “members” by “having produced some published results of
832 research in mineralogy, crystallography, or the allied sciences.”

833 This early alliance with the amateur community was a necessary concession
834 for the staff of the *American Mineralogist*, but the efforts to appeal to the collecting
835 community faded quickly as articles became more technical and the content more
836 arcane. In 1926, sensing that the professional community had usurped their
837 publication and a new journal was needed, Peter Zodak – an engineering inspector
838 for the Westchester County (NY) Park Commission – founded *Rocks and Minerals* to
839 service the collectors (Montgomery 1951). *Rocks and Minerals* has been joined by
840 *Lapidary Journal* (1947), the *Mineralogical Record* (1970), and other bulletins
841 targeted for amateur mineralogists (Neumeier, undated). MSA’s takeover of the
842 *American Mineralogist* was a statement of professional self-determination, allowing
843 US mineralogists to control the content of their publications, and in that fashion, to

844 define the boundaries of their science. But it also estranged MSA from those
845 enthusiasts who had sustained mineralogy over the previous century.

846

847 **Following Well-Trodden Paths to a New Mineral Society**

848 The emergence of the *American Mineralogist* was different from the genesis
849 of journals that originate in response to a paradigmatic discovery that inspires
850 proponents of the new vision to split from traditionalists. In our lifetimes,
851 innovations involving fractal geometry, nanoscience, astrobiology, and microbial
852 geochemistry offer examples of this latter pathway, and a host of new journals
853 dedicated to these subjects have appeared since 1990.

854 In contrast, the creation of the *American Mineralogist* – and the society that
855 supported it – was not disciplinarily groundbreaking. At least five countries can
856 boast continuously functioning mineralogical societies that are older than MSA: The
857 Russian Mineralogical Society (1817), which recently celebrated its *bicentennial*; the
858 Mineralogical Society of Great Britain and Ireland (1876); the French Society of
859 Mineralogy and Crystallography (1878); the Austrian Mineralogical Society (1901);
860 and the German Mineralogical Society (1908). Moreover, many of these associations
861 sponsored the publication of journals: *Zapiski RMO (Proceedings of the Russian*
862 *Mineralogical Society* since 1830); the Mineralogical Society's *Mineralogical*
863 *Magazine* (1876); and one can include the *European Journal of Mineralogy*, which in
864 1989 merged long-running mineralogical bulletins from France, Germany, Spain,
865 and Italy.

866 Even within the US, many specialized mineralogical societies had formed and
867 disappeared in the century before the formation of MSA. The history of these
868 evanescent groups is explored in Kraus (1921) and Greene and Burke (1978)⁴, but
869 three mineral collecting clubs that predate MSA are with us still: the New York
870 Mineralogical Club (1886); the Philadelphia Mineralogical Society (1892); and the
871 Newark (New Jersey) Mineralogical Society (1915). At the turn of the 19th century,
872 these three clubs served the needs of both professors and amateur collectors. They
873 held regular meetings with invited lecturers, and they published newsletters and
874 booklets to which professionals contributed.

875

876 **The Connection between the XRD Revolution and the MSA**

877 What convinced US mineralogists that the time had come to establish a
878 society organized and administered not by enthusiastic amateurs but by professors
879 of major universities? In his first presidential address, Kraus (1921) explicitly
880 acknowledges the X-ray diffraction revolution as sharing credit for the explosive
881 growth of the field, noting that mineralogy

882 “is no longer merely a descriptive science but by virtue of the development of
883 many quantitative methods and especially as the result of the epoch-making

⁴ The first mineralogical society in the US was founded in 1797 by Samuel Latham Mitchell, a professor at the College of Physicians and Surgeons in New York City. Named “The American Mineralogical Society” to promote “the investigation of the mineral and fossil bodies which compose the fabric of the Globe; and, more especially, for the natural and chemical history of the minerals and fossils of the United States,” its aim was “to arm every hand with a hammer, and every eye with a microscope” (Greene and Burke 1978). The AMS vanished in 1801.

884 discoveries in the field of crystal structure *it is now an exact science of*
885 *fundamental importance.* [Italics added]

886 Although American mineralogists were not yet actively engaged in X-ray diffraction
887 experiments, they recognized in the work of European physicists a seed that now
888 distinguished them from the more qualitative “geologists”.

889 In this regard, the proposal for a new society did not go far enough for
890 Frederick E. Wright of the Carnegie Geophysical Laboratory and for Prof. A.C. Gill of
891 Cornell University. As detailed in Phair (1969b), Wright and Gill believed that
892 crystallography was the *only* trait that differentiated MSA from GSA, and Wright
893 insisted on an organizational name change to “The Crystallographic Society of
894 America.” Gill concurred that “the crystallographic part was highly desirable” and
895 argued that “we need a *mineralogical* society as much as a cat needs three tails.”
896 Wright was a highly accomplished optical mineralogist, and he argued in a letter to
897 Kraus (Phair 1969b): “Crystallography is a much broader subject than mineralogy
898 and if we look upon crystallography as the science which has to deal with matter in
899 the crystal state then crystallography is on a par with physics and chemistry.”

900 The need to mollify Wright and Gill induced Kraus and Wherry to propose a
901 compromise title: The Crystallographical and Mineralogical Society of America.
902 This name appeared in the preliminary constitution and in a November 1919
903 announcement of the new society in *Science* (Fig. 20; Kraus et al. 1919). Wright’s
904 efforts did not survive the organizational meeting in December 1919 because, Phair

905 (1969b) speculates, the name was too cumbersome. But they elected Wright as
906 Councilor in an act of appeasement, and he eventually served as President in 1941.⁵

907 The emergence of the new crystallography from the realm of physics rather
908 than mineralogy was a double-edged sword for MSA's founders. On the one hand,
909 the idea that mineralogy is more closely affiliated with physics than geology offered
910 a quantitative rigor that justified a separation from GSA and the creation of a new
911 society. Indeed, one can argue that history repeated itself in the 1970s with the
912 emergence of "mineral physics" and the inauguration in 1977 of *Physics and*
913 *Chemistry of Minerals* to accommodate articles in high-pressure crystallography that
914 were not being accepted by the *American Mineralogist* (Charles Prewitt, pers.
915 comm.) On the other hand, the instrumental techniques to produce and detect X-
916 rays needed to be learned, and Ewald's invention of reciprocal space demanded a
917 sophisticated training in the mathematics of the scattering process.

918 Consequently, the first mineral structures to be solved in the US were the
919 work of physical chemists rather than mineralogists. Charles L. Burdick was a
920 graduate student at the Massachusetts Institute of Technology with Arthur A. Noyes,
921 soon afterward one of the founding fathers of Caltech. In 1914, Burdick snared a
922 compartment on the last German ocean liner to leave from New York for Hamburg
923 to pursue his Ph.D. research in Basel and Berlin. In early 1916, Burdick received a
924 letter from Noyes urging him to spend his final months in Europe with WH Bragg in

⁵ A Crystallographic Society of America with MSA representation was organized in 1939, suspended during the Second World War, and reinstated in 1946 (Notes and News, 1946). It merged with the American Society for X-Ray and Electron Diffraction in 1949 to create the American Crystallographic Association, which continues to thrive.

925 London because of Noyes's "strong belief in the importance of x-ray atomic
926 structure analysis for the future of theoretical chemistry, and his wish to get
927 something of the kind started at MIT (Burdick 1958)." Burdick returned to MIT,
928 built a Bragg X-ray spectrometer, then followed Noyes to Caltech and built another
929 spectrometer that was "probably the best of its day" (Burdick 1958). This
930 instrument enabled Burdick to collect high-quality data on a natural chalcopyrite
931 crystal from French Creek, PA, and he therewith published the first structure
932 determination of a mineral originating in the US (Burdick and Ellis 1917a,b).

933 Ralph Wyckoff received his doctorate in physics at Cornell under the tutelage
934 of Shoji Nishikawa, who himself had been trained in space group theory by Torahiko
935 Terada, "one of the few to work in Germany during the 1890s when the theory was
936 being created" (Wyckoff 1962). After Wyckoff received his degree in 1919, he
937 moved to the Carnegie Geophysical Laboratory "to begin there an application of X-
938 ray diffraction to minerals (Wyckoff 1962)," though he also studied artificial crystals
939 as well. Wyckoff revisited the structure of calcite and published XRD analyses of
940 rhodochrosite, magnesite, and siderite (Wyckoff 1920). Soon after, he published the
941 first structure for alabandite (MnS; Wyckoff 1921) and re-examined structures for
942 dolomite (Wyckoff and Merwin 1924) and cristobalite (Wyckoff 1925). Wyckoff
943 also collaborated with Herbert Merwin and Henry Washington of the Geophysical
944 Lab to standardize pyroxene terminology. Using a suite of minerals loaned by
945 William F. Foshag at the Smithsonian, they were first to observe that "all of the
946 different kinds of minerals usually grouped amongst the pyroxenes have the

947 structure of either diopside, enstatite, wollastonite, or rhodonite. (Wyckoff et al.
948 1925).”

949 Wyckoff’s eight years at the Geophysical Laboratory saw a prolific output of
950 natural and artificial crystal structure refinements as well as several treatises on
951 space group theory and general structure analysis. In 1927, however, he moved
952 away from geology to apply X-ray diffraction techniques to biological systems at the
953 Rockefeller Institute in New York. In a speech given to the Institute of Physics in
954 London nearly 30 years later, Wyckoff (1954) reflected that “[f]or the first 25 years
955 following the discovery of X-ray diffraction, there were very few in the United States
956 carrying out research in the subject.” He attributes the lag to several factors, of
957 which one was the recalcitrance of mineralogists:

958 “Our subject [i.e., crystallography] in America suffered severely from not
959 finding general acceptance as part of one branch of university science. With
960 us, crystallography has never been more than an occasional course given to
961 students of mineralogy, and our mineralogists were singularly slow in
962 realizing the value of X-ray methods.”

963 That is not a very generous characterization of the mineralogical community, nor is
964 it very accurate.

965 The record clearly shows that MSA members were highly attuned to the wall
966 of separation between physicists and mineralogists, and they were unhappy about
967 it. The Canadian MSA founder TL Walker (1923) laments, “Owing possibly to their
968 familiarity with the necessary technique and the possession of the laboratory
969 equipment, most of the work in this field [X-ray diffraction] up to the present time
970 has been carried on by physicists rather than by mineralogists.” In an assessment of

971 modern analytical techniques, Wyckoff's collaborator, H.S. Washington, explicitly
972 lauds his achievements (Washington 1925):

973 "Study of minerals along such lines is still in its infancy, but such examples as
974 have come under my notice lead to the conviction that X-ray methods,
975 especially when employed in conjunction with some of those longer known,
976 are not only the most recent but among the most powerful methods of
977 arriving at an understanding of what minerals, as well as artificial crystals,
978 really are, how they are constituted, and how they are related."

979 Arthur S. Eakle (1926), professor of mineralogy at the University of California-
980 Berkeley and MSA president in 1925, argued that mineralogical education needed to
981 be updated to include the new approaches in X-ray crystallography:

982 "The physicist with his superior electrical and instrumental knowledge has
983 devised instruments for important x-ray investigation of crystal structure
984 and mineral composition, and has substantiated the "space-lattice" theory of
985 internal molecular, or atomic, structure of crystals, and has been enabled to
986 make important additions to our knowledge of crystal symmetry. *We must*
987 *look to our crystallographers and mineralogists to carry on in this work since it*
988 *manifestly comes within their province; but there must be more of them to keep*
989 *pace with our modern methods of investigation.*" [Italics added]

990 These are not the musings of a community that was "singularly slow" in
991 appreciating the value of X-ray diffraction.

992 Instead, they reflect the reality that X-ray crystallography is a skill attained
993 through apprenticeship with expert practitioners. Burdick trained with the Braggs,
994 and Wyckoff was mentored by Nishikawa. And if mineralogists were ignorant of
995 physics, it is equally true that physicists were ignorant of mineralogy. The founders
996 of X-ray diffraction, von Laue and WL Bragg, admitted as much. In a posthumously
997 translated autobiographical remembrance, von Laue (1962) stated:

998 “Now, I had never studied mineralogy. During my first stay in Gottingen I had
999 made a halfhearted attempt to attend a mineralogy course but had given up
1000 very soon. From books I then learned the rudiments of crystallography, that
1001 is to say, crystal classes, that was all. The exam was administered by the
1002 geologist, Prof. Konen, and I still remember how his amusement grew and
1003 grew in the face of my entirely obvious ignorance until he finally broke off
1004 the interview.”

1005 In accepting the Roebling Medal from MSA in 1948, WL Bragg likewise expressed his
1006 surprise in receiving the recognition (Bragg 1949):

1007 “I am glad that you do not expect the recipient of the medal to pass a simple
1008 examination in mineralogy before he can accept his prize, for I am sure I
1009 would fail in that test. It is not merely a matter of knowing the subject, it is a
1010 deeper and more fundamental difference in outlook which divides the
1011 physicist from the mineralogist...

1012 “An exact scientist endeavours to simplify and generalize problems so that
1013 comparatively unequivocal decisions can be made. Followers of descriptive
1014 sciences such as mineralogy and petrology can never approach their problem
1015 from a one-sided standpoint, but must consider how products of nature came
1016 to be...”

1017 To a much greater degree than is true today, in the early decades of the twentieth
1018 century, the separate branches of the physical sciences were isolated, and crossing
1019 boundaries would take time.

1020 But not too much time. C.H. Stockwell, of the University of Wisconsin and
1021 then the Canadian Geological Survey, published the first XRD article in *The American*
1022 *Mineralogist* in 1927, on unit-cell parameters obtained from powder diffraction
1023 patterns of the garnet group (Stockwell 1927). The next year, John W. Gruner of the
1024 University of Minnesota published a technical article on the oscillation method for
1025 X-ray diffraction of crystals (Gruner 1928). Significant contributions to
1026 crystallography were developed by US scientists who made minerals a major part of

1027 their research: Linus Pauling, who won Nobel prizes in chemistry and peace; Martin
1028 Buerger, inventor of the precession camera; and JDH Donnay, who revealed
1029 relations between crystal form and atomic structure, among others. By the late
1030 1930s, *The American Mineralogist* offered about a half-dozen articles on X-ray
1031 crystallography of minerals each year. By the late 1940s, that increased to two
1032 dozen per year, and a decade later there are too many to count. These trends also
1033 are documented in Barton's (2019) data analysis of the ascension of X-ray
1034 diffraction in the discovery of new minerals from the 1930s to the 1970s.

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IMPLICATIONS

1037 **Reverberations of the XRD Revolution Today**

1038 The force with which mineralogists applied X-ray diffraction to extract the
1039 crystal structures of materials inspired an equal and opposite response as new
1040 techniques challenged our concepts of atomic order. Not surprisingly, incongruities
1041 between the classical model of crystallinity as conceived by the Braggs and the
1042 structural shortcomings exhibited by natural materials were recognized early. MSA
1043 founder Edgar T. Wherry, who first realized that bentonite is altered volcanic ash,
1044 was stymied by its classification. Are clays with intensive stacking disorder to be
1045 described as crystalline? Wherry (1925) argued that bentonite could be regarded as
1046 a "one-dimensional colloid." The semi-random intergrowths characteristic of illite-
1047 smectite mixtures continues to inspire new formalisms for the taxonomy of
1048 intermediate order (Moore and Reynolds 1997).

1049 The advent of high-resolution transmission electron microscopy shifted the
1050 focus from averaged atomic structures as deduced using X-rays to particular atomic
1051 configurations as resolved in micrographs. With this curtain drawn, the universality
1052 of nanoscale defects in natural materials became evident (Wenk 1976; Nieto and
1053 Livi 2013), and they came in myriad styles: layer-, chain- and tunnel-width disorder
1054 (Veblen and Buseck 1979; Turner and Buseck 1979; Veblen 1983); commensurate
1055 and incommensurate layer modulations (Drits 1987; Guggenheim and Eggleton
1056 1988); temperature- and strain-induced microtwins (Van Tendeloo et al. 1976;
1057 Goltrant et al. 1991); assorted line dislocations and ordered point defects (McLaren
1058 1991); fine-scale exsolution lamellae (Brown and Parsons 1984), and more. The
1059 observations of these microstructures posed a profound question regarding
1060 crystallinity: After how many unit-cells of repetitive stacking disorder, or
1061 superperiodic tunnel structures, or exsolution intergrowths, does the defect itself
1062 constitute a new mineral (Fig. 21)?

1063 These issues have grown even more pertinent in light of the most recent
1064 explorations of nanomaterials. As reviewed in the *American Mineralogist* Centennial
1065 article by Caraballo et al. (2015), in the last 25 years we have grown increasingly
1066 aware that the geochemistry of near-surface environments is controlled largely by
1067 nanophases (Fig. 22). The small dimensions of these particles yield high surface
1068 areas that can change their thermodynamic stabilities relative to the bulk
1069 (Navrotsky 2004), and the increased reactivity of the surfaces dramatically
1070 enhances their abilities to sorb and transport dissolved species or to promote redox
1071 or other chemical reactions (Hochella et al. 2008). These particles can grow through

1072 epitaxial attachment to form larger particles, requiring the introduction of states of
1073 intermediate crystallinity, sometimes termed mesocrystals (Cölfen and Antonietti
1074 2005). Characterizing the formation and evolution of these nanoparticles is at the
1075 heart of some of the most exciting science today, and it requires techniques that are
1076 themselves at the boundary between diffraction and spectroscopy, such as pair
1077 distribution function (PDF) analysis and synchrotron-based extended X-ray
1078 absorption spectroscopy (EXAFS) (O'Day et al. 1994; Michel et al. 2007).

1079 One hundred years ago, MSA materialized from a revolution that seemed
1080 finally to have resolved a most fundamental problem for Earth scientists: What do
1081 we mean when we say that a mineral is “crystalline”? A cutting edge of mineralogy
1082 today and for the foreseeable future is the exploration of the hypnagogic state for
1083 minerals: crystals that fall within that twilight zone between rigid order and atomic
1084 turmoil. Ironically, then, as MSA celebrates its centennial, we find ourselves
1085 revisiting the very problem whose solution inspired the Society’s birth.

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1087

ACKNOWLEDGMENTS

1088 The author acknowledges support from National Science Foundation Grant
1089 EAR1552211. Early drafts of this paper were greatly improved by stimulating
1090 discussions with and helpful comments by Charlie Burnham and Jeffrey Post. I also
1091 thank journal reviewers Charles Geiger and Keith Putirka, whose criticisms
1092 tightened the focus of the manuscript, and associate editor Warren Huff for handling
1093 this unusually long contribution.

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References

- 1095 Allen, E.T. (1916) The composition of natural bornite. American Journal of Science,
1096 245, 409-413.
- 1097 Armstrong, H.E. (1927) Poor common salt! Nature, 120, 478.
- 1098 Assmus, A. (1995) Early history of X-rays. Beam Line, 25, 10-24.
- 1099 Aulthier, A. (2004) Dynamical theory of X-ray diffraction. Oxford University Press,
1100 Oxford.
- 1101 Aulthier, A. (2013) Early Days of X-ray Crystallography. Oxford University Press,
1102 Oxford.
- 1103 Barlow, W. (1883) Probable nature of the internal symmetry of crystals. Nature, 29,
1104 186-188 and 205-207.
- 1105 Barlow, W. (1894) Über die Geometrischen Eigenschaften homogener starrer
1106 Strukturen und ihre Anwendung auf Krystalle. Zeitschrift für
1107 Krystallographie und Minerologie, 23, 1-63.
- 1108 Barlow, W. and Pope, W.J. (1906) A development of the atomic theory which
1109 correlates chemical and crystalline structure and leads to a demonstration of
1110 the nature of valency. Journal of the Chemical Society, Transactions, 89,
1111 1675-1744.
- 1112 Barlow, W. and Pope, W.J. (1907) The relation between the crystalline form and the
1113 chemical constitution of simple inorganic substances. Journal of the
1114 Chemical Society, Transactions, 91, 1150-1177.
- 1115 Barton, I. (2019) Trends in the discovery of new minerals over the last century.
1116 American Mineralogist, 104, 641-651.

- 1117 Bates, A.C. (1916) Arthur Chamberlain and his magazines. *American Mineralogist*, 1,
1118 1-2.
- 1119 Bayley, W.S. (1910) *Elementary Crystallography*. McGraw-Hill Book Company, New
1120 York.
- 1121 Berzelius, J.J. (1814) *Attempt to Establish a Pure Scientific System of Mineralogy by*
1122 *the Application of the Electro-Chemical Theory and the Chemical*
1123 *Proportions*. Translated by John Black. C. Baldwin, London.
- 1124 Berzelius, J.J. (1824) Om de förändringar i det kemiska Mineralsystemet, som blifva
1125 en nödvändig följd af isomorpha kroppars egenskap att ersätta hvarandra i
1126 obestämda förhållanden. *Konglig Vetenskaps-Academiens Handlingar*, 112-
1127 142
- 1128 Blackmore, J.T. (1972) *Ernst Mach: His Work, Life, and Influence*. University of
1129 California Press, Berkeley.
- 1130 Bohr, N. (1913) I. On the constitution of atoms and molecules. *The London,*
1131 *Edinburgh, and Dublin Philosophical Magazine and Journal of Science*, 26, 1-
1132 25.
- 1133 Boscovich, R.G. (1758) *Philosophiae naturalis theoria redacta ad unicum legem*
1134 *virium in natura existentium*. Prostat Viennae Austriae, Officina Libraria
1135 Kaliwodiana.
- 1136 Bragg, W. H. (1912) X-rays and crystals. *Nature*, 90, 219.
- 1137 Bragg, W.H. and Bragg, W.L. (1913) The structure of the diamond. *Proceedings of*
1138 *the Royal Society of London. Series A*, 89, 277-291.

- 1139 Bragg, W.H. and Bragg, W.L. (1915) X-rays and Crystal Structure. G. Bell and Sons,
1140 London.
- 1141 Bragg, W. L. (1912) The specular reflection of X-rays. *Nature*, 90, 410.
- 1142 Bragg, W.L. (1913a) The diffraction of short electromagnetic waves by a crystal.
1143 *Proceedings of the Cambridge Philosophical Society*. 17, 43-57.
- 1144 Bragg, W.L. (1913b) The structure of some crystals as indicated by their diffraction
1145 of X-rays. *Proceedings of the Royal Society of London Series A*, 89, 248-277.
- 1146 Bragg, W.L. (1914) The analysis of crystals by the X-ray spectrometer. *Proceedings*
1147 *of the Royal Society of London Series A*, 90, 468-489.
- 1148 Bragg, W.L. (1949) Acceptance of the Roebling Medal of the Mineralogical Society of
1149 America. *American Mineralogist*, 34, 238-241.
- 1150 Bragg, W.L. (1962) Personal reminiscences. In Ewald, P.P., Ed. *Fifty Years of X-ray*
1151 *Diffraction*. International Union of Crystallography, Glasgow. pp. 531-539.
- 1152 Bravais, A. (1851) *Etudes cristallographiques*. *Journal de l'Ecole Polytechnique*, 20,
1153 101-276.
- 1154 Brock, W.H. and Knight, D.M. (1965) The atomic debates: "Memorable and
1155 interesting evenings in the life of the Chemical Society. *Isis*, 56, 5-25.
- 1156 Brown, C. M. (2014). *Benjamin Silliman: A life in the young republic*. Princeton
1157 University Press, Princeton, N.J.
- 1158 Brown, W. L. and Parsons, I. (1984) The nature of potassium feldspar, exsolution
1159 microtextures and development of dislocations as a function of composition
1160 in perthitic alkali feldspars. *Contributions to Mineralogy and Petrology*, 86,
1161 335-341.

- 1162 Bruce, A. (1968) The American Mineralogical Journal. Contributions to the History
1163 of Geology, vol. 1. Hafner Publishing, New York.
- 1164 Brush, S.G. (1968) Mach and atomism. *Synthese*, 18, 192-215.
- 1165 Buddington, A.F. (1937) Memorial of Alexander Hamilton Phillips. *American*
1166 *Mineralogist*, 22, 1094-1098.
- 1167 Buerger, M.J. (1990) Brief history of structure determination. In Lima-de-Faria, Ed.,
1168 *Historical Atlas of Crystallography*, Kluwer Academic Publishers, Dordrecht,
1169 pp. 109-123.
- 1170 Burdick, C.L. (1958) The genesis and beginnings of X-ray crystallography at Caltech.
1171 *Physics Today*, 11, 20.
- 1172 Burdick, C.L. and Ellis, J.H. (1917a) The crystal structure of chalcopyrite determined
1173 by X-rays. *Journal of the American Chemical Society*, 39, 2518-2525.
- 1174 Burdick, C.L. and Ellis, J.H. (1917b) The crystal structure of chalcopyrite determined
1175 by X-rays. *Proceedings of the National Academy of Sciences*, 3, 644-649.
- 1176 Caraballo, M.A., Michel, F.M. and Hochella Jr, M.F. (2015). The rapid expansion of
1177 environmental mineralogy in unconventional ways: Beyond the accepted
1178 definition of a mineral, the latest technology, and using nature as our guide.
1179 *American Mineralogist*, 100, 14-25.
- 1180 Chalmers, A. (2014) Atomism from the 17th to the 20th Century. In Zalta, E.N., Ed.,
1181 *The Stanford Encyclopedia of Philosophy*, URL
1182 <<https://plato.stanford.edu/archives/win2014/entries/atomism-modern/>>.
- 1183 Christidis, G.E., and Huff, W.D. (2009). Geological aspects and genesis of bentonites.
1184 *Elements*, 5, 93-98.

- 1185 Cölfen, H. and Antonietti, M. (2005) Mesocrystals: inorganic superstructures made
1186 by highly parallel crystallization and controlled alignment. *Angewandte*
1187 *Chemie International Edition*, 44, 5576-5591.
- 1188 Dalton, J. (1808) *A New System of Chemical Philosophy*. S. Russell, Manchester.
- 1189 Dana, E.S. (1912) *A Textbook of Mineralogy*. John Wiley and Sons, New York.
- 1190 Dana, J.D. (1837) *A System of Mineralogy*. Durrie & Peck and Herrick & Noyes, New
1191 Haven.
- 1192 Dana, J.D. (1845) Observations on pseudomorphism. *American Journal of Science*
1193 *and Arts*, 48, 81-92.
- 1194 Dana, J.D. (1854) *A System of Mineralogy*, 4th Ed. George. P. Putnman, New York.
- 1195 Dana, J.D. and Brush, G.J. (1869) *A System of Mineralogy*, 5th Ed. John Wiley and Son,
1196 New York.
- 1197 Darwin, C.G. (1914) The theory of X-ray reflexion. *Philosophical Magazine*, 27, 315-
1198 333 and 675-690.
- 1199 Debye, P. (1913) Über den Einfluss der Wärmebewegung auf die
1200 Interferenzerscheinungen bei Röntgenstrahlen, *Verhandlungen der*
1201 *Deutschen Physikalischen Gesellschaft*, 15, 678-689.
- 1202 Debye, P. and Scherrer, P. (1916) Interferenz an regellos orientierten Teilchen im
1203 Röntgenlicht. I. *Physikalische Zeitschrift*, 17, 277-283.
- 1204 Drits V.A. (1987) SAED and HREM Study of Order/Disorder and Structural
1205 Heterogeneity in Layer Minerals. In Drits, Ed. *Electron Diffraction and High-*
1206 *Resolution Electron Microscopy of Mineral Structures*. Springer, Berlin,
1207 Heidelberg, pp. 217-238.

- 1208 Eakle, A.S. (1926) Needed extension in mineralogic instruction. American
1209 Mineralogist, 11, 45-52.
- 1210 Eckert, M. (2012). Disputed discovery: the beginnings of X-ray diffraction in crystals
1211 in 1912 and its repercussions. Acta Crystallographica Section A: Foundations
1212 of Crystallography, 68(1), 30-39.
- 1213 Ewald, P.P. (1913) Zur Theorie der Interferenzen der Röntgenstrahlen in Kristallen.
1214 Physikalische Zeitschrift, 14, 465-472.
- 1215 Fleck, G.M. (1963) Atomism in late nineteenth-century physical chemistry. Journal of
1216 the History of Ideas, 24, 106-114.
- 1217 Ford, W.E. and Bradley, W.M. (1916a). Margarosanite, a new lead-calcium silicate
1218 from Franklin, New Jersey. American Journal of Science, 248, 159-162.
- 1219 Ford, W.E. and Bradley, W.M. (1916b) On hydro-zincite. American Journal of Science,
1220 247, 59-62.
- 1221 Forman, P. (1969). The discovery of the diffraction of X-rays by crystals; a critique of
1222 the myths. Archive for History of Exact Sciences, 6, 38-71.
- 1223 Frankenheim, M. L. (1826). Crystallonomische Aufsätze. ISI Enzyklopadische
1224 Zeitung Oken, 5, 497-515 and 542-565.
- 1225 Friedel, G. (1913) Sur les symmetries cristallines que peut reveler la diffraction des
1226 rayons Röntgen. Comptes Rendus de l'Académie des Sciences, 157, 1533-
1227 1536.
- 1228 Friedrich, W., Knipping, P. and von Laue, M.T. F. (1912) interferenz-Erscheinungen
1229 bei Röntgenstrahlen. Sitzungsberichte der Mathematischen-Physikalischen

- 1230 Klasse der Königlich Bayerischen Akademie der Wissenschaften zu München,
1231 303-322.
- 1232 Friedrich, W., Knipping, P., and Laue, M. (1913) Interferenzerscheinungen bei
1233 roentgenstrahlen. *Annalen der Physik*, 346, 971-988.
- 1234 Gadolin, A.V. (1867) Deduction of all crystallographic systems and their subdivisions
1235 by means of a single general principle. (In Russian) *Annals of the Imperial St*
1236 *Petersburg Mineralogical Society Series 2*, 4, 112-200.
- 1237 Geiger, C.A. (2016) A tale of two garnets: The role of solid solution in the
1238 development toward a modern mineralogy. *American Mineralogist*, 101,
1239 1735-1749.
- 1240 Gibbs, J.W. (1902) *Elementary Principles in Statistical Mechanics Developed with*
1241 *Especial Reference to the Rational Foundation of Thermodynamics.*
1242 *Scribner's Sons, New York.*
- 1243 Gibson, C.S. (1941) Sir William Jackson Pope 1870-1939. *Obituary Notices of*
1244 *Fellows of the Royal Society*, 3, 291-324.
- 1245 von Gliszczynski, S. and Stoicovici, E. (1938) Beitrag zum Melanophlogitproblem.
1246 *Zeitschrift für Kristallographie-Crystalline Materials*, 99, 238-250.
- 1247 Goltrant, O., Cordier, P. and Doukhan, J.C. (1991) Planar deformation features in
1248 shocked quartz; a transmission electron microscopy investigation. *Earth and*
1249 *Planetary Science Letters*, 106, 103-115.
- 1250 Gordin, M.D. (2019) *A Well-Ordered Thing: Dmitrii Mendeleev and the Shadow of*
1251 *the Periodic Table.* Princeton University Press, Princeton, NJ.
- 1252 Gordon, S.G. (1917) *Proceedings of Societies.* *American Mineralogist*, 2, 68.

- 1253 Grabowski, J.J. (1992) Sports in Cleveland: an illustrated history. Case Western
1254 Reserve University, Cleveland.
- 1255 Greene, J.C. and Burke, J. G. (1978). The science of minerals in the age of Jefferson.
1256 Transactions of the American Philosophical Society, 68, 1-113.
- 1257 Grossman, M.I. (2017) John Dalton and the origin of the atomic theory: reassessing
1258 the influence of Bryan Higgins. The British Journal for the History of Science,
1259 50, 657–676.
- 1260 Groth, P. (1906) An Introduction to Chemical Crystallography. John Wiley and Sons,
1261 New York.
- 1262 Gruner, J.W. (1928) The oscillation method of X-ray analysis of crystals. American
1263 Mineralogist, 3, 123-141.
- 1264 Guggenheim, S. and Eggleton, R.A. (1988) Crystal chemistry, classification, and
1265 identification of modulated layer silicates. Reviews in Mineralogy and
1266 Geochemistry, 19, 675-725.
- 1267 Hales, T. C. (2005). A proof of the Kepler conjecture. Annals of Mathematics, 1065-
1268 1185.
- 1269 Hausmann, J.F.L. (1813) Handbuch der Mineralogie. 3 volumes, Göttingen. Second
1270 edition. pp. 302.
- 1271 Haüy-R.-J. (1784) Essai d'une Théorie sur la structure des Crystaux. Gougué and Née
1272 de la Rochelle, Paris.
- 1273 Haüy, R.J. (1801) Traité de Minéralogie. Council of Mines, Paris.
- 1274 Heaney, P. J. (2016). Time's arrow in the trees of life and minerals. *American*
1275 *Mineralogist*, 101(5), 1027-1035.

- 1276 Hessel, J.F.C. (1830) Krystall. In Gehler's Physikalisches Wörterbuch, 5, 1023-1360.
1277 Schwickert, Leipzig. Reprinted in W.F. Ostwald (1897). Klassiker der exacten
1278 Wissenschaften, 89, 41-124.
- 1279 Hochella, M.F., Lower, S.K., Maurice, P.A., Penn, R.L., Sahai, N., Sparks, D.L. and
1280 Twining, B.S. (2008) Nanominerals, mineral nanoparticles, and earth
1281 systems. Science, 319, 1631-1635.
- 1282 Hooke, R. (1665) Micrographia: or some physiological descriptions of minute bodies
1283 made by magnifying glasses with observations and inquiries made
1284 thereupon. Jo. Martyn and Ja. Allestry, Royal Society, London.
- 1285 Hooker, M. and Montgomery, A. (1975) Edgar Theodore Wherry. American
1286 Mineralogist, 60, 533-539.
- 1287 Hull, A. W. (1917a). A new method of X-ray crystal analysis. Physical Review, 10,
1288 661-697.
- 1289 Hull, A.W. (1917b) The crystal structure of iron. Physical Review, 9, 84-87.
- 1290 Hull, A.W. (1922) The crystal structures of the common elements. Journal of the
1291 Franklin Institute, 189-216.
- 1292 Hull, A.W. (1946) Thirty years of X-ray research at the General Electric Research
1293 Laboratory. American Journal of Physics, 14, 71-79.
- 1294 Hunt, W.F. (1955) Edward Henry Kraus. American Mineralogist, 40, 945-951.
- 1295 Hunt, W.F. and Kraus, E.H. (1916). Note on the variable composition of
1296 melanochalcite. American Journal of Science, 242, 211-214.
- 1297 Hunter, G.K. (2004). Light is a messenger: the life and science of William Lawrence
1298 Bragg. Oxford University Press.

- 1299 Huygens, C. (1690) *Traité de la lumière*. Pieter van der Aa, Leiden.
- 1300 Jackson, J. (2005) *A World on Fire*. Viking Press, New York.
- 1301 James, R.W. (1948). *The Optical Principles of the Diffraction of X-rays*. G. Bell and
1302 Sons, London.
- 1303 Johnson, S. (2008) *The Invention of Air*. Riverhead Books, New York.
- 1304 Kaji, M. (2002) D.I. Mendeleev's concept of the chemical elements and *The Principles*
1305 *of Chemistry*. *Bulletin for the History of Chemistry*, 27, 4-16.
- 1306 Kargon, R. (1965). Mendeleev's chemical ether, electrons, and the atomic theory.
1307 *Journal of Chemical Education*, 42, 388-389.
- 1308 Kean, S. (2011) *The Disappearing Spoon*. Little, Brown, and Company, New York.
- 1309 Kepler, J. (1611) *Strena seu de nive sexangula*. Gottfried Tampach, Frankfurt.
- 1310 Kolata, D.R., Huff, W.D., and Bergstrom, S.M. (1996). Ordovician K-bentonites of
1311 eastern North America (Vol. 313). Geological Society of America.
- 1312 Kraus, E.H. (1919) *Crystallographical and Mineralogical Society of America*. *Science*,
1313 50, 497.
- 1314 Kraus, E.H. (1921) The future of mineralogy in America. *American Mineralogist*, 6,
1315 23-34.
- 1316 Kraus, E.H., and Hunt, W.F. (1920). *Mineralogy: An Introduction to the Study of*
1317 *Minerals and Crystals*. McGraw-Hill book Company, Inc., New York.
- 1318 Kraus, E.H. (1934) Memorial of Frank Robertson Van Horn. *American Mineralogist*,
1319 19, 101-105.
- 1320 Kubbinga, H. (2012) *Crystallography from Haüy to Laue: Controversies on the*
1321 *molecular and atomistic nature of solids*. *Acta Crystallographica A*, 68, 3-29.

- 1322 Kuhn, T. (1996) *The Structure of Scientific Revolutions*. University of Chicago Press,
1323 Chicago.
- 1324 Lalena, J.N. (2006) From quartz to quasicrystals: probing nature's geometric
1325 patterns in crystalline substances. *Crystallography Reviews*, 12, 125-180.
- 1326 Langmuir, I. (1919) The arrangement of electrons in atoms and molecules. *Journal*
1327 *of the American Chemical Society*, 41, 868-934.
- 1328 von Laue, M. (1912) *Eine quantitative Prüfung der Theorie für die Interferenz-*
1329 *Erscheinungen bei Röntgenstrahlen*. Verlag der Königlichen Bayerische
1330 Akademie der Wissenschaften, 363-373.
- 1331 von Laue, M. (1962) My development as a physicist: An autobiography. In Ewald,
1332 P.P., Ed. *Fifty Years of X-ray Diffraction*. International Union of
1333 Crystallography, Glasgow. pp. 278-307.
- 1334 Levison, W.G. (1917) *Proceedings of Societies*. *American Mineralogist*, 2, 67-68.
- 1335 Lewis, G.N. (1908). The osmotic pressure of concentrated solutions, and the laws of
1336 the perfect solution. *Journal of the American Chemical Society*, 30, 668-683.
- 1337 Lewis, G.N. (1916). The atom and the molecule. *Journal of the American Chemical*
1338 *Society*, 38, 762-785.
- 1339 Lewis, G.N. (1926). The conservation of photons. *Nature*, 118, 874-875.
- 1340 Lima-de-Faria, J. (1990) Time-maps of crystallography. In Lima-de-Faria, Ed.,
1341 *Historical Atlas of Crystallography*, Kluwer Academic Publishers, Dordrecht,
1342 pp. 5-42.
- 1343 Lindley, D. (2015) *Boltzmann's Atom: The Great Debate that Launched a Revolution*
1344 *in Physics*. The Free Press, New York.

- 1345 Mach, E. (1883) Die Mechanik ihrer Entwicklung. F.A. Brockhaus, Leipzig.
- 1346 Mach, E. (1919) The Science of Mechanics. Trans. McCormack, T.J. Open Court
1347 Publishing, Chicago.
- 1348 Madelung, E. (1909) Molekulare Eigenschwingungen. Nachrichten von der
1349 Gesellschaft der Wissenschaften zu Göttingen, Mathematisch-Physikalische
1350 Klasse, 100-106.
- 1351 McLaren, A.C. (1991) Transmission electron microscopy of minerals and rocks.
1352 Cambridge University Press, Cambridge.
- 1353 Melhado, E.M. (1980) Mitscherlich's discovery of isomorphism. Historical Studies in
1354 the Physical Sciences, 11, 87-123.
- 1355 Melhado, E.M. (1981) Jacob Berzelius: The Emergence of his Chemical System.
1356 University of Wisconsin Press, Madison. Cambridge University Press,
1357 Cambridge.
- 1358 Melhado, E.M. and Frdnsgmyr, T., Eds. (2003) Enlightenment science in the romantic
1359 era: The chemistry of Berzelius and its cultural setting (Vol. 10). Cambridge
1360 University Press, Cambridge.
- 1361 Mendeleev, D. (1879). The periodic law of the chemical elements. The Chemical
1362 News, 40, No. 1042.
- 1363 Mendeleev, D. (1891) Principles of Chemistry, Vol 1. Translated by G. Kamensky,
1364 Longmans, Green & Co., London.
- 1365 Michel, F.M., Ehm, L., Antao, S.M., Lee, P.L., Chupas, P.J., Liu, G., Strongin, D.R.,
1366 Schoonen, M.A., Phillips, B.L. and Parise, J.B. (2007) The structure of
1367 ferrihydrite, a nanocrystalline material. Science, 316, 1726-1729.

- 1368 Miers, H.A. (1902) *Mineralogy: An Introduction to the Scientific Study of Minerals*.
1369 MacMillan and Co., London.
- 1370 Miers, H.A. (1918) The old and the new mineralogy. *Journal of the Chemical Society*,
1371 *Transactions*, 113, 363-386.
- 1372 Mitscherlich, E. (1819) Über die Kristallisation der Salze, in denen das Metall der
1373 Basis mit zwei Proportionen Sauerstoff verbunden ist. *Abhandlungen*,
1374 *Akademie der Wissenschaften*, Berlin, pp. 427-437.
- 1375 Mitscherlich, E. (1821) Über das Verhältniss zwischen der chemischen
1376 Zusammensetzung und der Krystallform arseniksaurer und phosphorsaurer
1377 Salze. W. Engelmann, Leipzig.
- 1378 Mitscherlich, E. (1822) Sur la relation qui existe entre la forme crystalline et les
1379 proportions chimiques. I. Mémoire sur les arseniates et les phosphates.
1380 *Annales des Chimie et des Physique* 19, 350-419.
- 1381 Montgomery A. (1951) Peter Zodac and *Rocks and Minerals*. *Rocks & Minerals*, 26,
1382 451-453.
- 1383 Moore, D.M. and Reynolds, R.C. Jr. (1997) *X-ray diffraction and the identification and*
1384 *analysis of clay minerals*. 2nd Ed. Oxford University Press, Oxford.
- 1385 Moore, P.B. (1990) Brief history of chemical crystallography. I. Inorganic
1386 compounds. In Lima-de-Faria, Ed., *Historical Atlas of Crystallography*, Kluwer
1387 Academic Publishers, Dordrecht, pp. 5-42.
- 1388 Morrow, S.I. (1969) One hundred and fifty years of isomorphism. *Journal of*
1389 *Chemical Education*, 46, 580-583.

- 1390 Moseley, H.G.J. (1913) The high-frequency spectra of the elements. Philosophical
1391 Magazine, 26, 1024-1034.
- 1392 Moses, A.J. and Parsons, C.L. (1900) Elements of Mineralogy, Crystallography and
1393 Blowpipe Analysis. 2nd Ed. D. Van Nostrand Company, New York.
- 1394 Moses, A.J. and Parsons, C.L. (1916) Elements of Mineralogy, Crystallography and
1395 Blowpipe Analysis. 5th Ed. D. Van Nostrand Company, New York.
- 1396 Navrotsky, A. (2004). Energetic clues to pathways to biomineralization: Precursors,
1397 clusters, and nanoparticles. Proceedings of the National Academy of Sciences,
1398 101, 12096-12101.
- 1399 Neumeier, G. A brief history of mineral magazines. Newsletter of the New York
1400 Mineralogical Club.
1401 [http://www.newyorkmineralogicalclub.org/history/minutes/Introduction%](http://www.newyorkmineralogicalclub.org/history/minutes/Introduction%20--%20A%20Brief%20History%20of%20Mineral%20Magazines.pdf)
1402 [20--%20A%20Brief%20History%20of%20Mineral%20Magazines.pdf](http://www.newyorkmineralogicalclub.org/history/minutes/Introduction%20--%20A%20Brief%20History%20of%20Mineral%20Magazines.pdf)
- 1403 Niaz, M., Rodríguez, M.A., and Brito, A. (2004) An appraisal of Mendeleev's
1404 contribution to the development of the periodic table. Studies in the History
1405 and Philosophy of Science, 35, 271-282.
- 1406 Nieto, F. and Livi, K.J. (Eds.). (2013). Minerals at the Nanoscale (Vol. 14). The
1407 Mineralogical Society of Great Britain and Ireland.
- 1408 Notes and News (1946) The Crystallographic Society. American Mineralogist, 31, 84.
- 1409 O'Day, P.A., Rehr, J.J., Zabinsky, S.I. and Brown, G.J. (1994) Extended X-ray
1410 absorption fine structure (EXAFS) analysis of disorder and multiple-
1411 scattering in complex crystalline solids. Journal of the American Chemical
1412 Society, 116, 2938-2949.

- 1413 Ostwald, W. (1904) Faraday Lecture: Elements and compounds. Journal of the
1414 Chemical Society, Transactions, 85, 506-522.
- 1415 Parsons, A.L. (1943) Memorial of Thomas Leonard Walker. American Mineralogist,
1416 28, 167-173.
- 1417 Pauling, L. (1929) The principles determining the structure of complex ionic
1418 crystals. Journal of the American Chemical Society, 51, 1010-1026.
- 1419 Perutz M.F. (1990) How W.L. Bragg invented X-ray analysis. Acta Crystallographica
1420 A, 46, 633-643.
- 1421 Pfeiffer, P. (1917) Crystals as molecular compounds. Zeitschrift für anorganische
1422 chemie. 97, 161-174.
- 1423 Phair, G. (1969a) The American Mineralogist: Its first four years. American
1424 Mineralogist, 54, 1233-1243.
- 1425 Phair, G. (1969b) The founding of the Mineralogical Society of America. American
1426 Mineralogist, 54, 1244-1255.
- 1427 Phillips, A.H. (1912) Mineralogy: An Introduction to the Theoretical and Practical
1428 Study of Minerals. MacMillan, New York.
- 1429 Phillips, A.H. (1916) New zinc phosphates from Salmo, B. C. American Journal of
1430 Science, 249, 275-278.
- 1431 Pojman, P. (2011) Ernst Mach. In Zalta, E.N., Ed., The Stanford Encyclopedia of
1432 Philosophy. URL:
1433 <<https://plato.stanford.edu/archives/win2011/entries/ernst-mach/>>.
- 1434 Pope, W.J. (1935) William Barlow 1845-1934. Obituary Notices of Fellows of the
1435 Royal Society, 1, 367-370.

- 1436 Pough, F.H. (1949) Memorial of Herbert Percy Whitlock. *American Mineralogist*, 34,
1437 261-266.
- 1438 Rhodes, R. (1986) *The making of the atomic bomb*. Simon and Schuster, New York.
- 1439 Rogers, A.F. (1921) *Introduction to the Study of Minerals and Rocks*. McGraw-Hill
1440 Book Co., New York.
- 1441 Rutherford, E. (1911) The Scattering of α and β Particles by Matter and the
1442 Structure of the Atom. *Philosophical Magazine*. 21, 669–688.
- 1443 Senechal, M. (1990) Brief history of geometrical crystallography. In Lima-de-Faria,
1444 Ed., *Historical Atlas of Crystallography*, Kluwer Academic Publishers,
1445 Dordrecht, pp. 43-59.
- 1446 Smits, A. and Scheffer, F.E.C. (1917) The interpretation of the “Roentgenograms” and
1447 Roentgen spectra of crystals. *Proceedings of the Koninklijke Akademie van*
1448 *Wetenschappen te Amsterdam*, 19, 432-338.
- 1449 Solly, R.H. (1894) *An Elementary Introduction to Mineralogy*. C.J. Clay and Sons,
1450 London.
- 1451 Sohncke, L. (1888). Erweiterung der Theorie der Krystallstructur. *Zeitschrift für*
1452 *Kristallographie-Crystalline Materials*, 14, 426-446.
- 1453 Stockwell, C.H. (1927) An X-ray study of the garnet group. *American Mineralogist*,
1454 12, 327-344.
- 1455 Taber, S. (1916) The growth of crystals under external pressure. *American Journal*
1456 *of Science*, 246, 532-556.
- 1457 Thomson, J.J. (1904). On the structure of the atom: an investigation of the stability
1458 and periods of oscillation of a number of corpuscles arranged at equal

- 1459 intervals around the circumference of a circle; with application of the results
1460 to the theory of atomic structure. *Philosophical Magazine*, 7, 237-265.
- 1461 Turner, S. and Buseck, P.R. (1979). Manganese oxide tunnel structures and their
1462 intergrowths. *Science*, 203, 456-458.
- 1463 Van Melsen, A.G. (1960) From atomos to atom: the history of the concept atom.
1464 Harper and Brothers, New York.
- 1465 Van Tendeloo, G., Van Landuyt, J. and Amelinckx, S. (1976). The $\alpha \rightarrow \beta$ phase
1466 transition in quartz and $AlPO_4$ as studied by electron microscopy and
1467 diffraction. *Physica Status Solidi (A)*, 33, 723-735.
- 1468 Veblen, D.R. (1983) Microstructures and mixed layering in intergrown wonesite,
1469 chlorite, talc, biotite, and kaolinite. *American Mineralogist*, 68, 566-580.
- 1470 Veblen, D.R. and Buseck, P.R. (1979) Chain-width order and disorder in
1471 biopyriboles. *American Mineralogist*, 64, 687-700.
- 1472 Walker, T.L. (1923) The development of mineralogical methods. *American*
1473 *Mineralogist*, 8, 41-46.
- 1474 Washington, H.S. (1925) The modern study of minerals. *American Mineralogist*, 10,
1475 45-52.
- 1476 Weiss, C.S. (1814) Uebersichliche Darstellung des verschie- denen naturlichen
1477 Abteilungen der Kristallisationssysteme. *Abhandlungen der Koniglichen*
1478 *Akademie der Wissenschaften in Berlin*, 289-344.
- 1479 Wenk, H.-R., Ed. (1976) *Electron Microscopy in Mineralogy*. Springer-Verlag, Berlin.
- 1480 Wherry, E.T. (1917a). Clay derived from volcanic dust in the Pierre in South Dakota.
1481 *Journal of the Washington Academy of Sciences*, 7, 576-583.

- 1482 Wherry, E.T. (1917b) Review of two recent papers on crystal structure. American
1483 Mineralogist, 2, 36-38
- 1484 Wherry, E.T. (1918) Abstracts of crystallographic literature. American Mineralogist,
1485 3, 137-147.
- 1486 Wherry, E.T. (1925) Bentonite as a one-dimensional colloid. American Mineralogist,
1487 10, 120-123.
- 1488 Whitlock, H.P. (1920) The Mineralogical Society of America. Science, 51, 219-220.
- 1489 Wollaston, W.H. (1812) On the primitive crystals of carbonate of lime, bitter-spar,
1490 and iron-spar. Philosophical Transactions of the Royal Society of London,
1491 102, 159-162.
- 1492 Wollaston, W.H. (1813) The Bakerian Lecture: On the elementary particles of certain
1493 crystals. Philosophical Transactions of the Royal Society of London, 103, 51-
1494 63.
- 1495 Wooster, W.A. (1990) Brief history of physical crystallography. In Lima-de-Faria, J.,
1496 Ed. Historical Atlas of Crystallography, Kluwer Academic Publishers,
1497 Dordrecht, pp. 61-75.
- 1498 Wyckoff, R.W.G. (1920). The crystal structures of some carbonates of the calcite
1499 group. American Journal of Science, 299, 317-360.
- 1500 Wyckoff, R.W.G. (1921). The crystal structure of alabandite (MnS). American Journal
1501 of Science, 11, 239-249.
- 1502 Wyckoff, R.W. (1925) Crystal structure of high temperature cristobalite. American
1503 Journal of Science, 54, 448-459.

- 1504 Wyckoff, R.W.G. (1954) Some thoughts on the future of natural science, with
1505 illustrations from the growth of X-ray diffraction work in the United States.
1506 British Journal of Applied Physics, 5, 199-204.
- 1507 Wyckoff, R.W.G. (1962) Reminiscences. In Ewald, P.P., Ed. Fifty Years of X-ray
1508 Diffraction. International Union of Crystallography, Glasgow. pp. 691-694.
- 1509 Wyckoff, R.W.G. and Merwin, H.E. (1924) The crystal structure of dolomite.
1510 American Journal of Science, 48, 447-461.
- 1511 Wyckoff, R.W., Merwin, H.E., and Washington, H.S. (1925). X-ray diffraction
1512 measurements upon the pyroxenes. American Journal of Science, 59, 383-
1513 397.
- 1514
- 1515

1516 Figure Captions

1517

1518 Figure 1: The Six Founders of MSA. A) Edward H. Kraus (from MSA Centennial
1519 website); B) Alexander H. Phillips (from Am Min Obit); C) Frank R. Van Horn
1520 (From Am Min obit); D) Thomas L. Walker (from Am Min obit); F) Edgar T.
1521 Wherry (from MSA web page).

1522

1523 Figure 2: A) René Just Haüy (engraving by Ambroise Tardieu) (open source from
1524 Wikipedia); B) Construction of pentagonal dodecahedron of pyrite by
1525 integrant molecules from *Traité de Mineralogie* (1801). (from Wikimedia
1526 commons)

1527

1528 Figure 3: A) Closest packing of atoms in a snowflake from Keppler's *Strena Seu de*
1529 *Nive Sexangula* (1611) [from Google Books]; B) Drawings of quartz crystals
1530 and their component "globular bodies" from Hooke's *Micrographia*
1531 *Restaurata* (1665) [from Google Books]; C) Arrangement of spherical bodies
1532 to explain cleavage angles in calcite from Huygens *Traité de la Lumière*
1533 (1690) [from Google Books].

1534

1535 Figure 4: William Wollaston's (1813) proposed construction of Haüy's polyhedral
1536 *molécules intégrantes* using spheres and ellipsoids. [Open access article]

1537

1538 Figure 5: The “Father of Atomic Theory” John Dalton (1808) correlated chemical
1539 with physical atomicity. Part 1 in this figure represents the arrangement of
1540 “particles” in water, and Parts 2, 5, and 6 portray the geometrical constraints
1541 of particles in ice. [From open access article]

1542

1543 Figure 6: A) William Barlow and B) William Jackson Pope [terms of [https:// about](https://about.jstor.org/terms)
1544 [jstor.org/terms](https://about.jstor.org/terms)]

1545

1546 Figure 7: Schemes for closest packing of spheres in crystals from Barlow (1883).
1547 [From Nature Publishing Group]

1548

1549 Figure 8: Barlow’s (1898) model for cubic closest packed spheres with smaller
1550 spheres tangentially located within interstices. [From Zeitschrift für
1551 Kristallographie]

1552

1553 Figure 9: A) Dmitri Mendeleev (1834-1907); B) Ernst Mach (1838-1916). [From
1554 Wikipedia]

1555

1556 Figure 10: Photograph of Max von Laue (1879-1960) [from Wikipedia]

1557

1558 Figure 11: A) First X-ray diffraction pattern of copper sulfate [from [http://what-](http://what-when-how.com/proteomics/history-and-future-of-x-ray-structure-)
1559 [when-how.com/proteomics/history-and-future-of-x-ray-structure-](http://what-when-how.com/proteomics/history-and-future-of-x-ray-structure-)

1560 [determination-proteomics/](#)]; B) First published X-ray diffraction pattern of
1561 sphalerite (Friedrich et al. 1913).

1562

1563 Figure 12: A) William Lawrence Bragg (1890-1971) (left) and William Henry Bragg
1564 (1862-1942) (right) (Acc. 90-105 - Science Service, Records, 1920s-1970s,
1565 Smithsonian Institution Archives). [Reprinted according to fair use copyright
1566 laws]. B) Reflection of X-ray pencils from parallel planes within crystal to
1567 generate diffraction spots (Bragg 1913a).

1568

1569 Figure 13: A) Ernest Rutherford (1831-1937); B) Niels Bohr (1885-1962) [From
1570 Wikipedia]

1571

1572 Figure 14: A) Paul Ewald (1888-1985) [from JSTOR archives]; B) Representation of
1573 X-ray scattering sphere in reciprocal space from Ewald (1913) [From
1574 *Physikalische Zeitschrift* from Hathitrust.org]

1575

1576 Figure 15: Founders of *The American Mineralogist*: A) Samuel G. Gordon (1897-
1577 1952); B) Harry W. Trudell (1880-1964) [both from Mineralogical Record
1578 online archives]

1579

1580 Figure 16: A) Gilbert N. Lewis (1875-1946) [from Wikipedia]; B) Dot notation for
1581 H₂O, HI, and I₂ from Lewis (1916) [from Journal of the American Chemical
1582 Society]

1583

1584 Figure 17: Wherry's (1918) representations of the structures of A) diamond and B)
1585 body-centered cubic structures such as α -Fe. Note his inferred physical
1586 shapes of the atoms required by the unit-cell geometries to the right. [From
1587 Wherry 1918 in Am Min]

1588

1589 Figure 18: Lewis's sketches for the disposition of valence electrons around "cubical
1590 atoms," formalized in Lewis (1916). [From Wikipedia]

1591

1592 Figure 19: The Founders' Letter circulated in 1917. [From MSA Centennial website]

1593

1594 Figure 20: The announcement in the Nov. 28, 1919 issue of *Science* of the founding
1595 of the "Crystallographical and Mineralogical Society of America." [From
1596 Science magazine]

1597

1598 Figure 21: Aperiodic fine (A) and coarse (B) slabs in mixed-layer chlorite ("C")-mica
1599 ("M") intergrowths with c^* horizontal. Inset diffraction patterns show heavy
1600 streaking along $00l$ due to the fine intergrowths. Diagram at bottom shows
1601 the structure of the nonconventional setting for the C (chlorite) and M (mica)
1602 slabs outlined in HRTEM images. Reprinted from Veblen (1983). [From Am
1603 Min article]

1604

1605 Figure 24: Transmission electron microscope images of synthetic akaganeite (γ -
1606 FeOOH) nanoparticles. Published with permission of Kris Peterson.



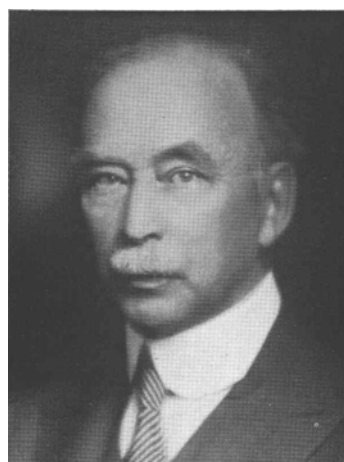
Edward H. Kraus (1875-1973)



Alexander H. Phillips (1866-1937)



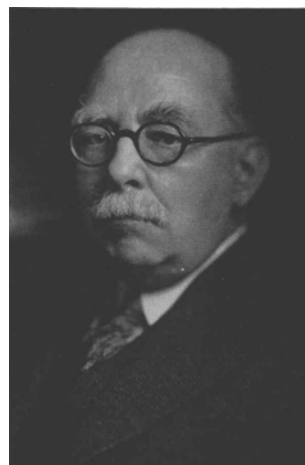
Frank R. Van Horn (1872-1933)



Thomas L. Walker (1867-1942)



Edgar T. Wherry (1885-1982)



Herbert P. Whitlock (1868-1948)

Figure 1: The six founders of MSA.

A



René Just Haüy (1743-1822)

B

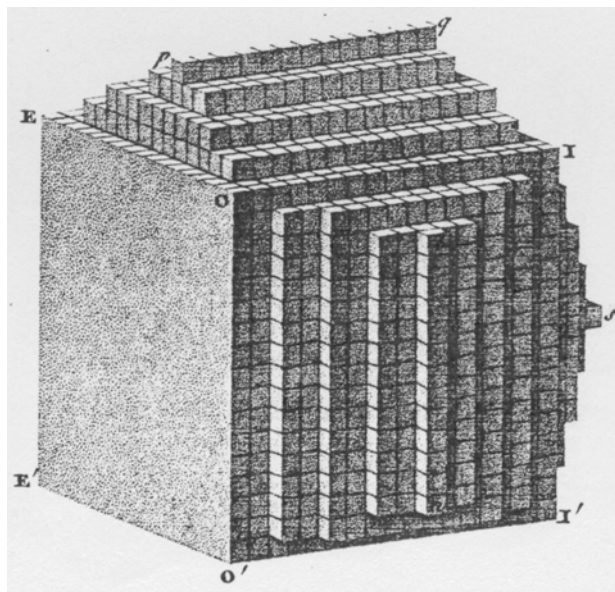


Figure 2: A) René Just Haüy (engraving by Ambroise Tardieu); B) Construction of pentagonal dodecahedron of pyrite by integrant molecules from *Traité de Mineralogie* (1801).

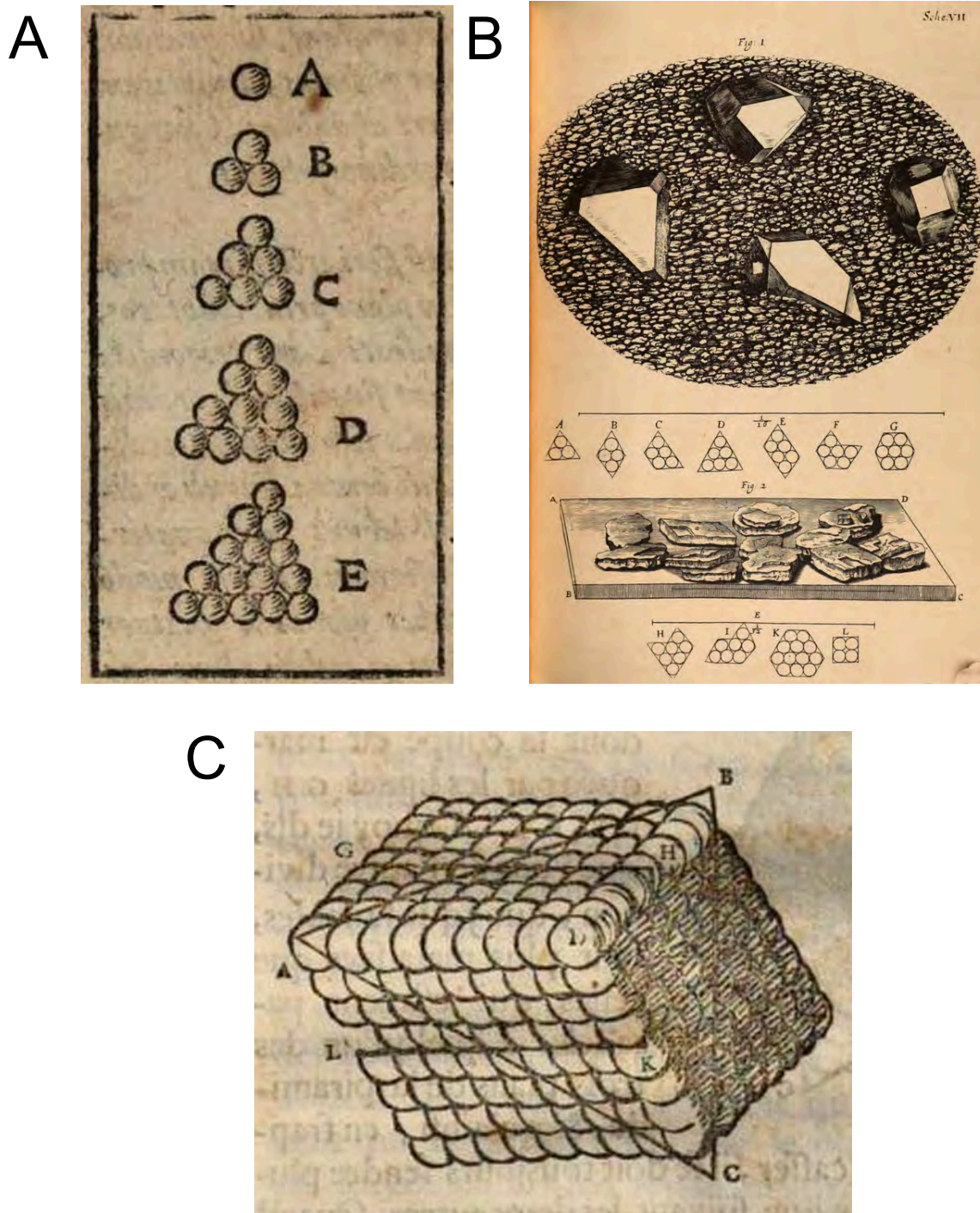


Figure 3: A) Closest packing of atoms in a snowflake from Kepler's *Strena Seu de Nive Sexangula* (1611); B) Drawings of quartz crystals and their component "globular bodies" from Hooke's *Micrographia Restaurata* (1665); C) Arrangement of spherical bodies to explain cleavage angles in calcite from Huygens *Traité de la Lumière* (1690).

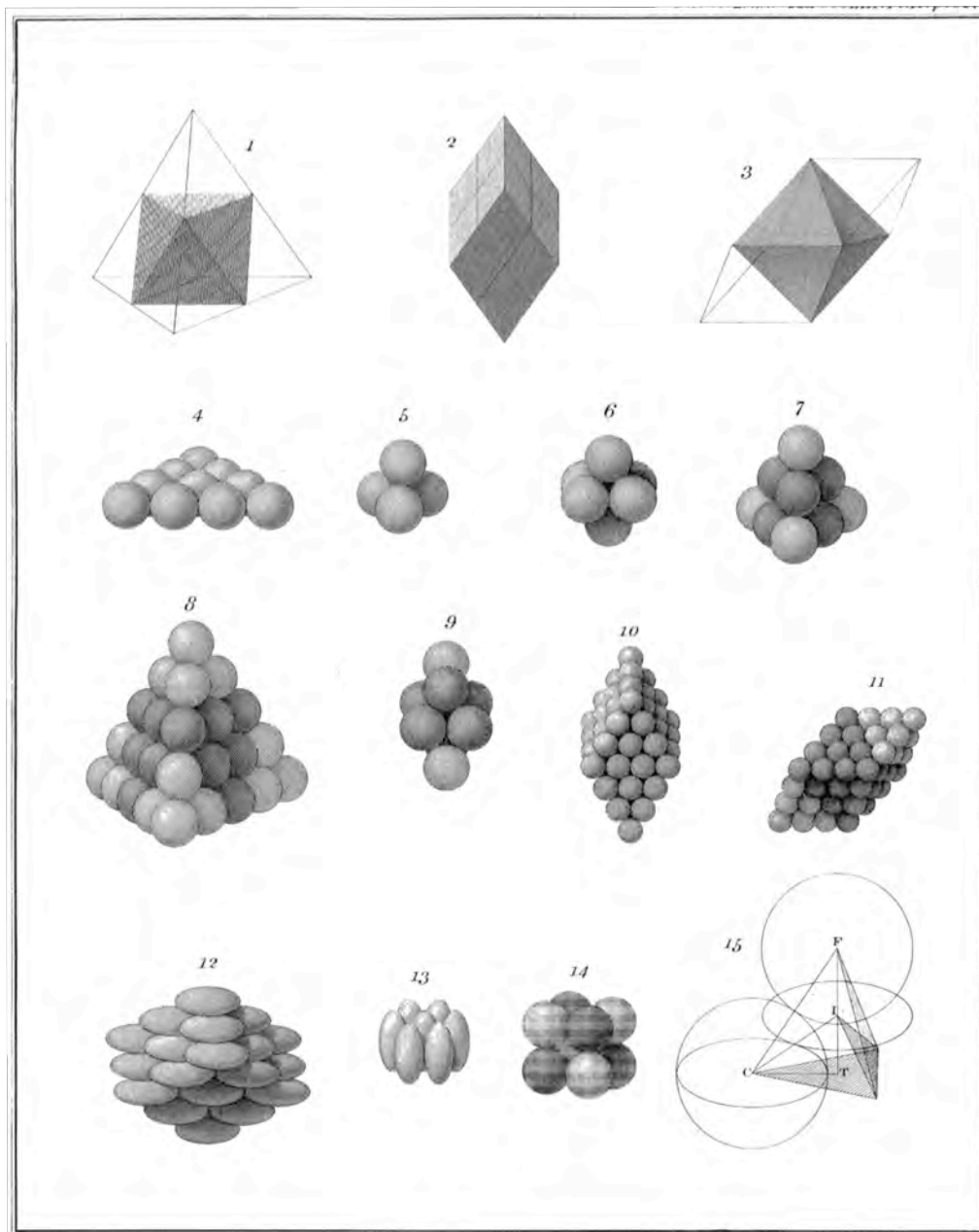


Figure 4: William Wollaston's (1813) proposed construction of Haüy's polyhedral *molécules intégrantes* using spheres and ellipsoids. [Open access]

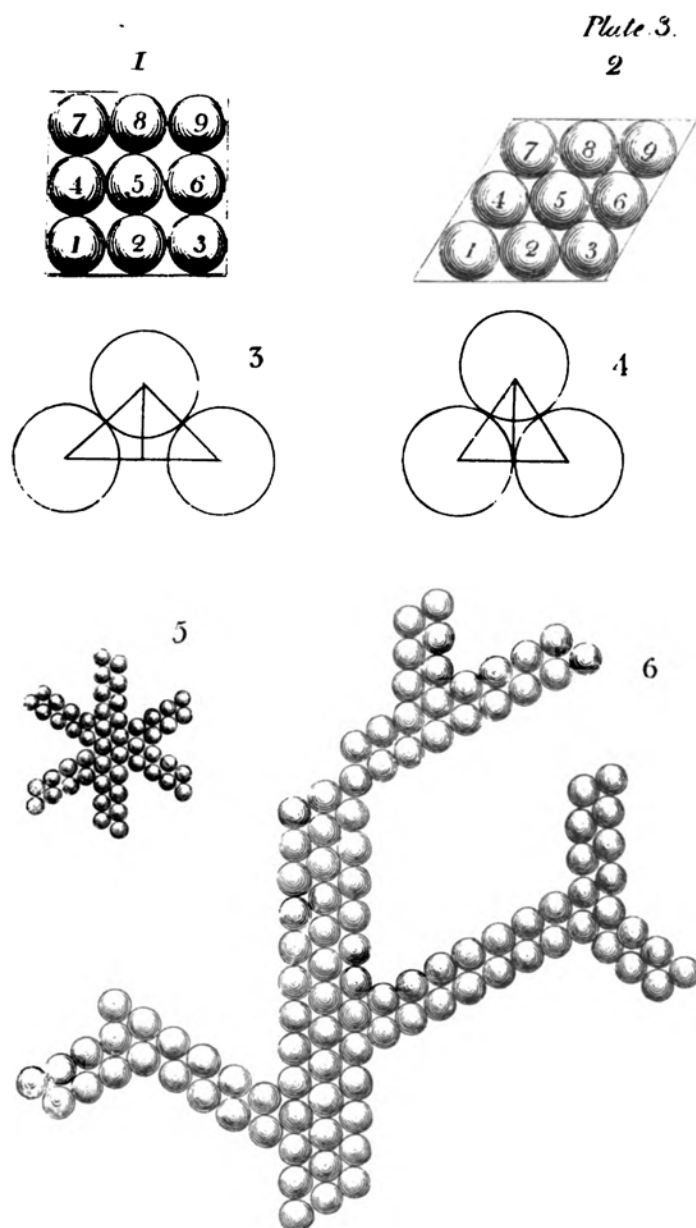
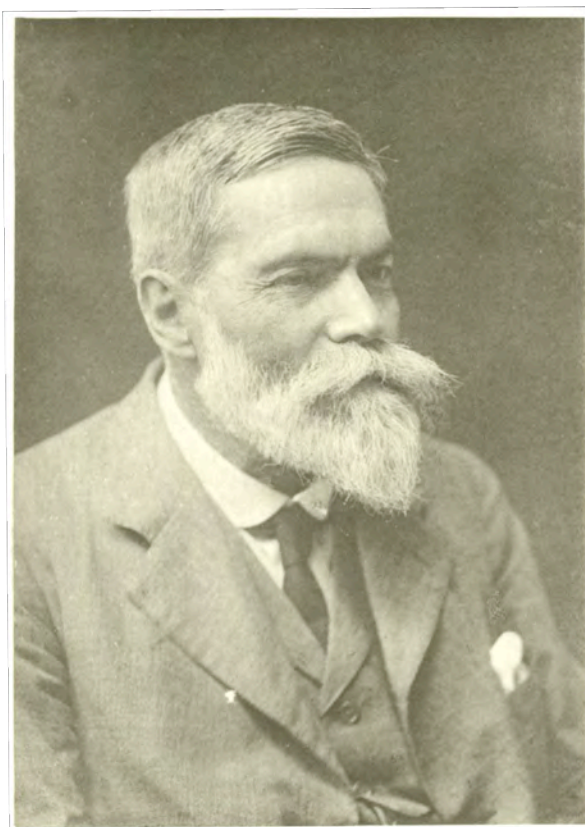
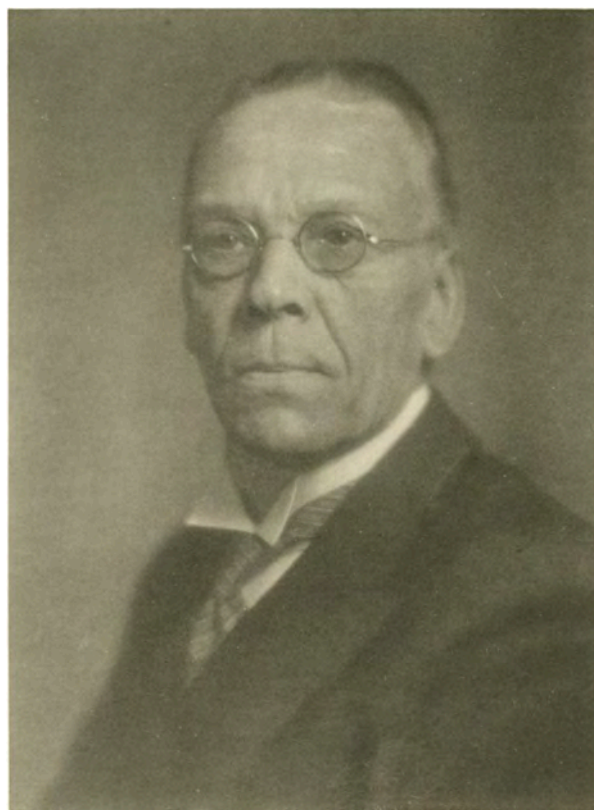


Figure 5: The “Father of Atomic Theory” John Dalton (1808) correlated chemical with physical atomicity. Part 1 in this figure represents the arrangement of “particles” in water, and Parts 2, 5, and 6 portray the geometrical constraints of particles in ice.



William Barlow (1845-1934)



William Jackson Pope (1870-1939)

Figure 6: William Barlow and William Jackson Pope

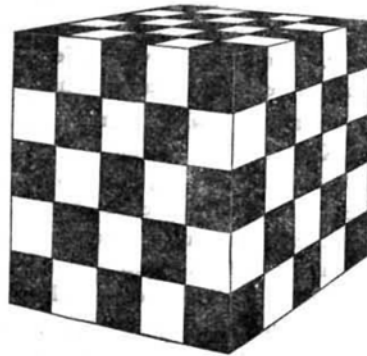


FIG. 1.

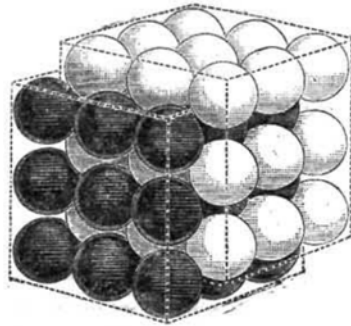
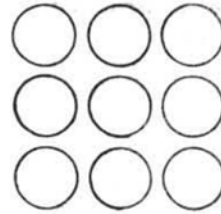


FIG. 2.



Plan α .

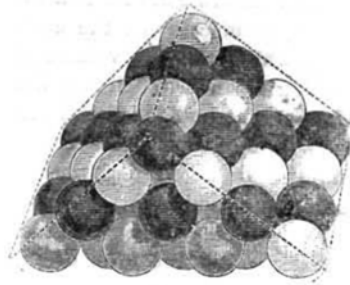
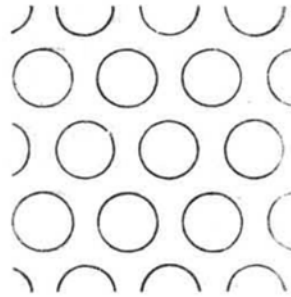


FIG. 3.



Plan β .

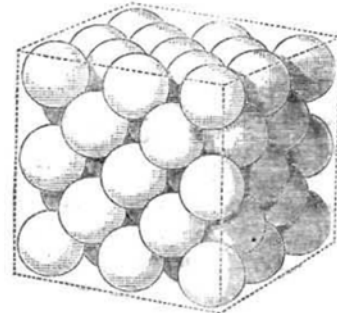
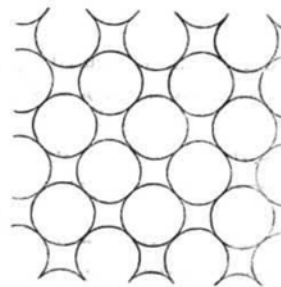


FIG. 4.



Plan γ .

Figure 7: Schemes for closest packing of spheres in crystals from Barlow (1883).

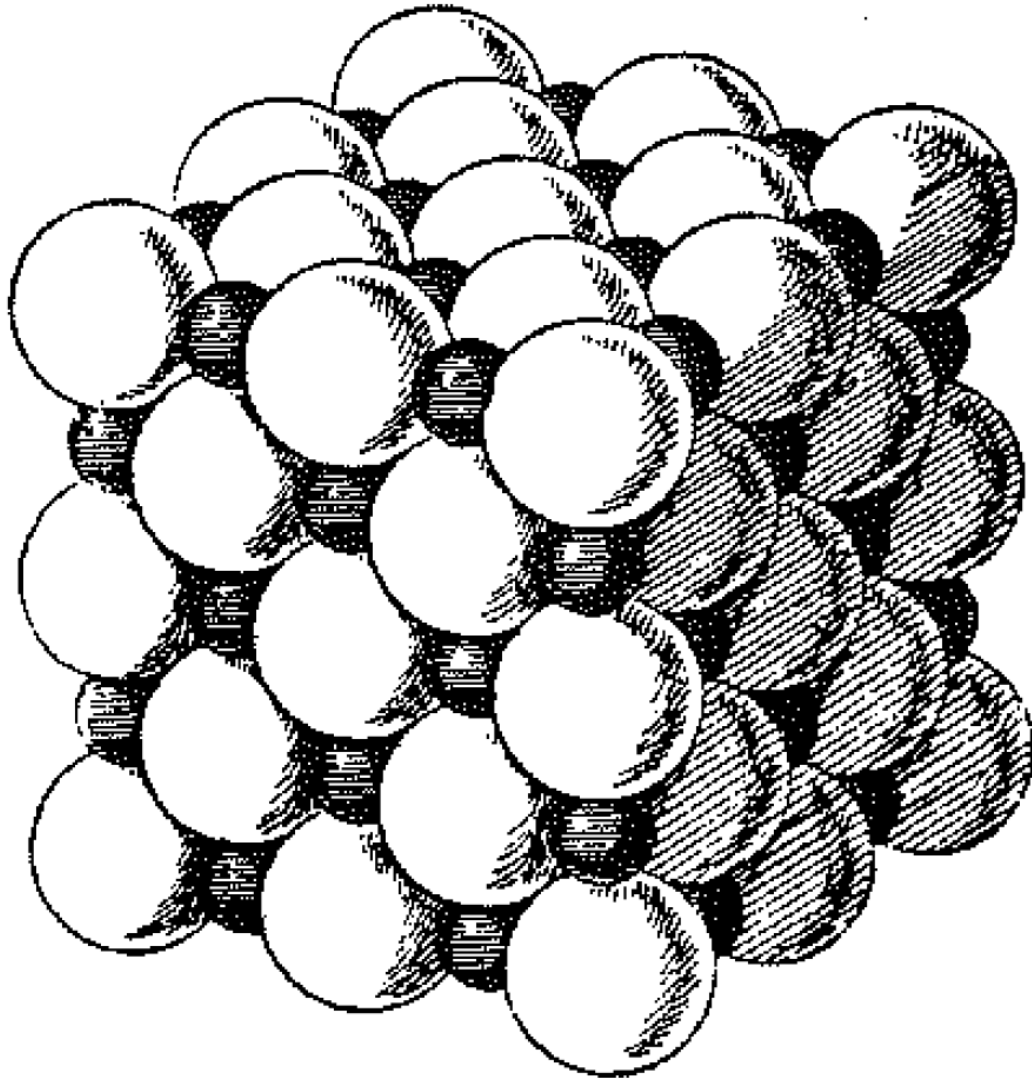


Figure 8: Barlow's (1898) model for cubic closest packed spheres with smaller spheres tangentially located within interstices.

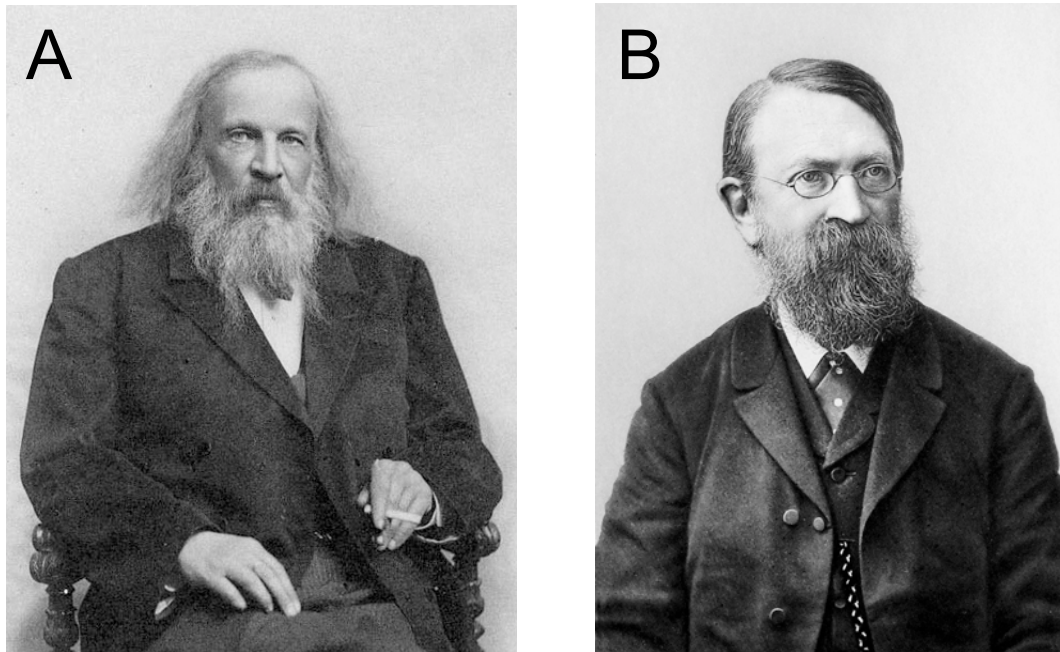
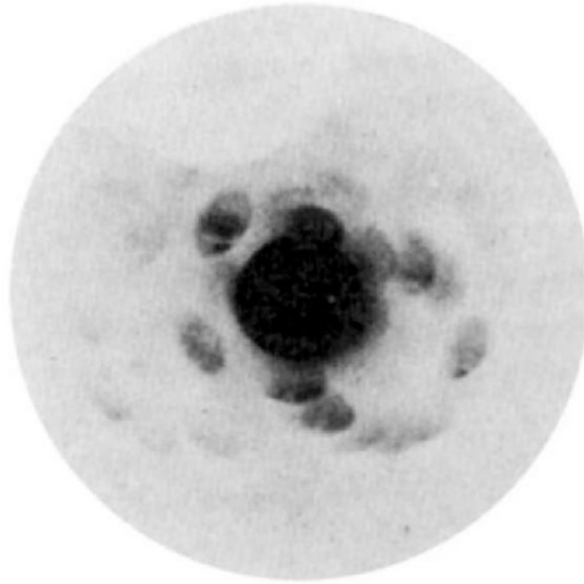


Figure 9: A) Dmitri Mendeleev (1834-1907); B) Ernst Mach (1838-1916).



Figure 10: Max von Laue (1879-1960)

A



B

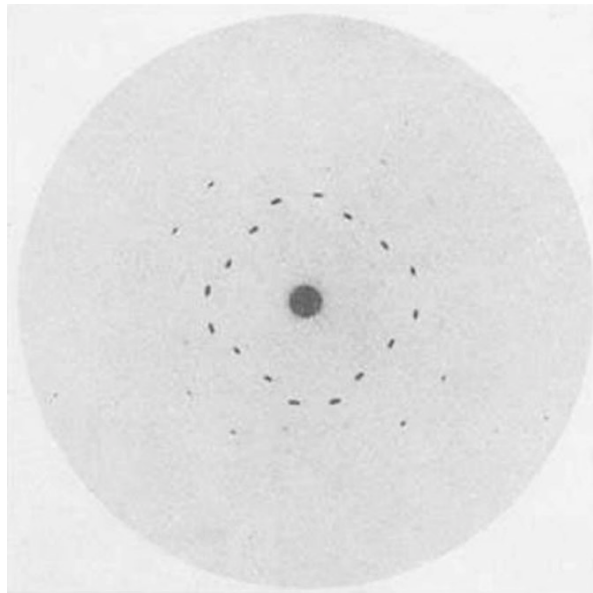


Figure 11: A) First X-ray diffraction pattern of copper sulfate; B) First X-ray diffraction pattern of sphalerite (Friedrich et al. 1913).

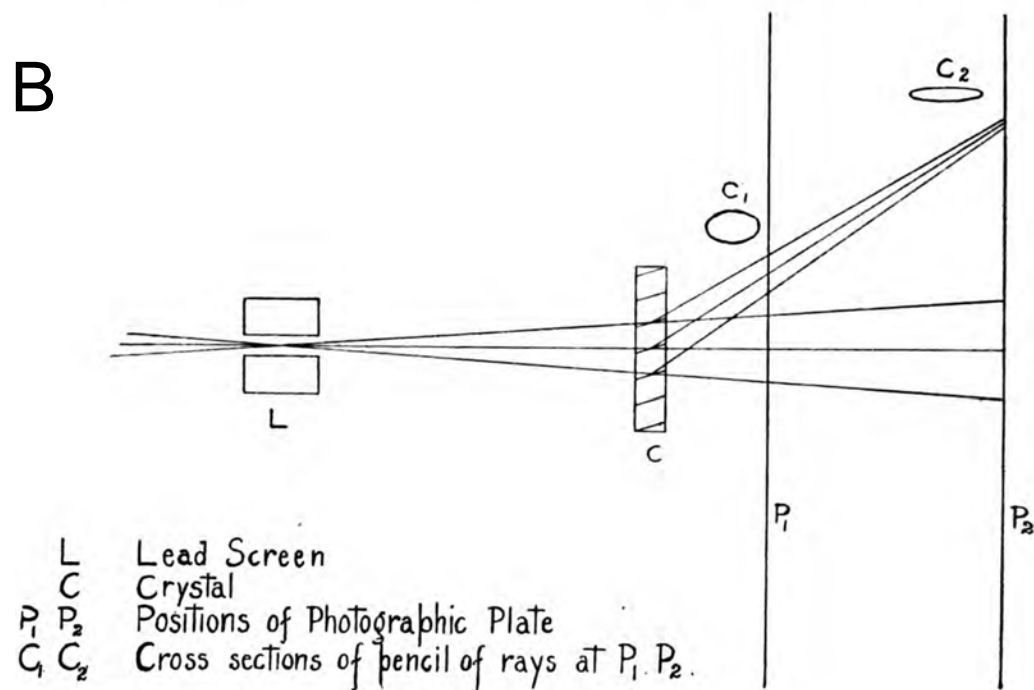
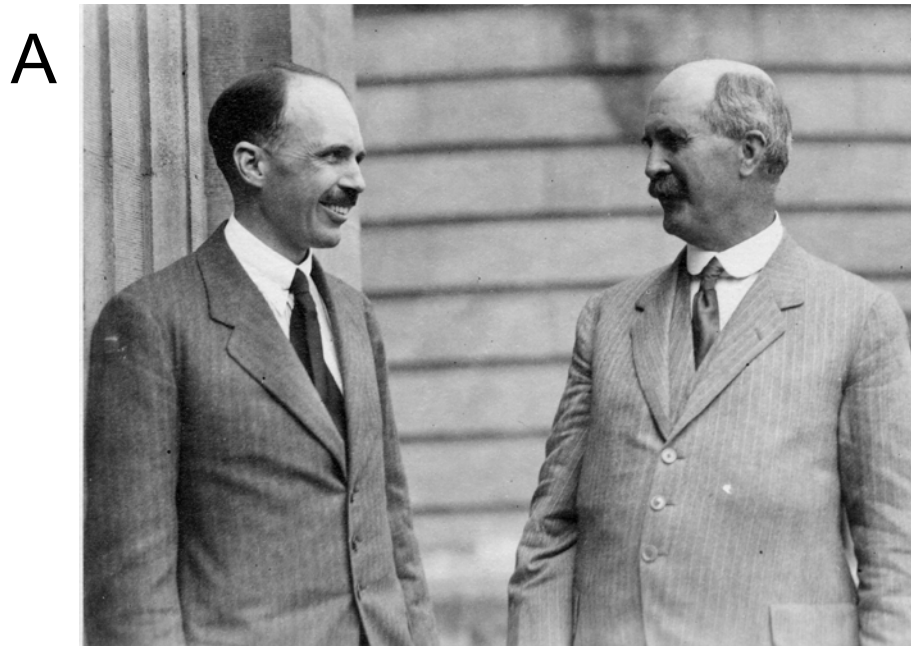


FIG. 2.

Figure 12: A) William Lawrence Bragg (1890-1971) (left) and William Henry Bragg (1862-1942) (right) (Acc. 90-105 - Science Service, Records, 1920s-1970s, Smithsonian Institution Archives). B) Reflection of X-ray pencils from parallel planes within crystal to generate diffraction spots (Bragg 1913a).

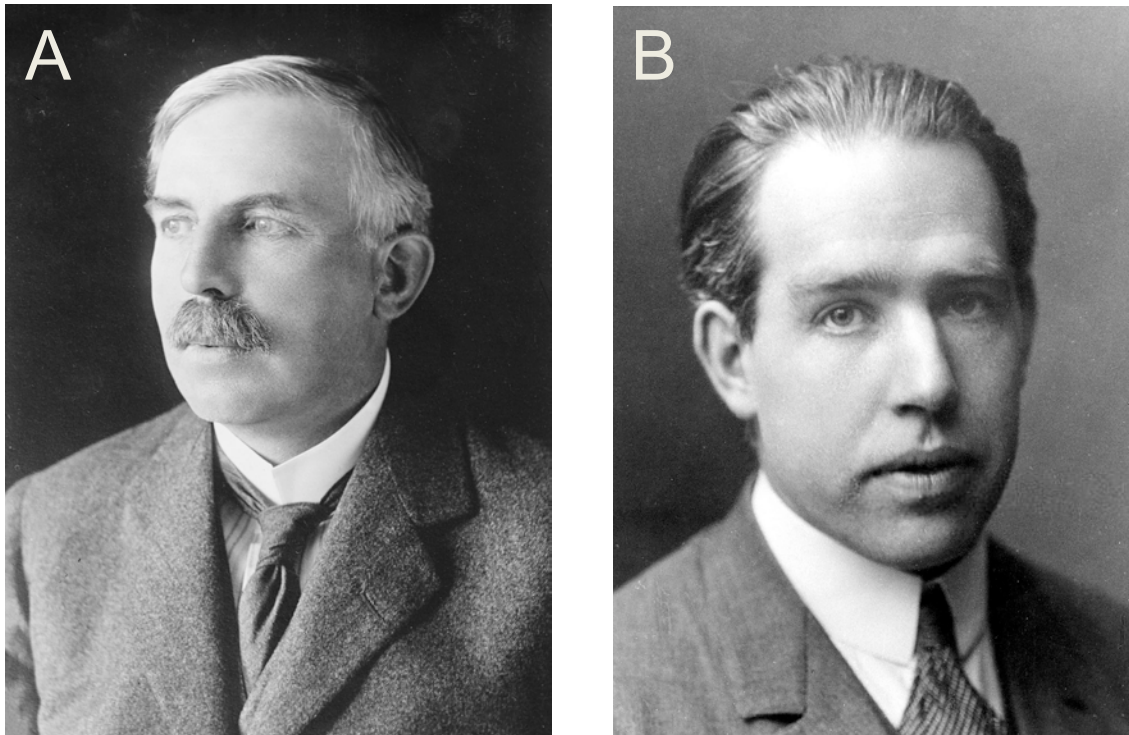
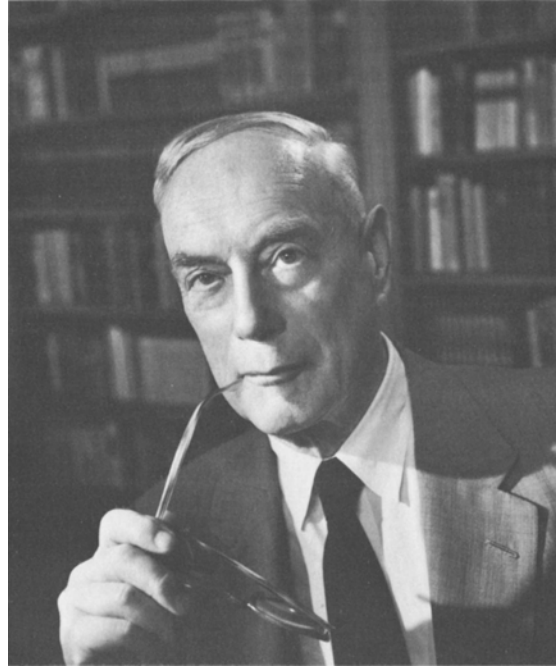


Figure 13: A) Ernest Rutherford (1831-1937); B) Niels Bohr (1885-1962)

A



B

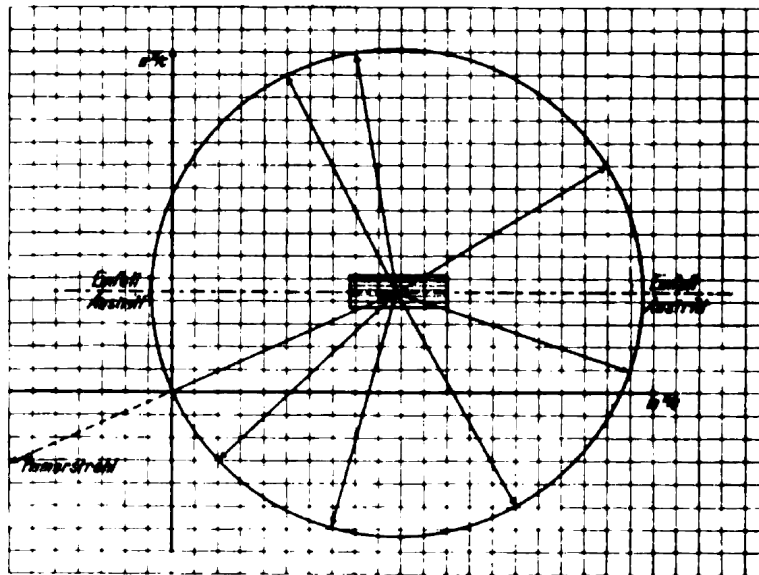


Figure 14: A) Paul Ewald (1888-1985); B) Representation of X-ray scattering sphere in reciprocal space from Ewald (1913)

A



B

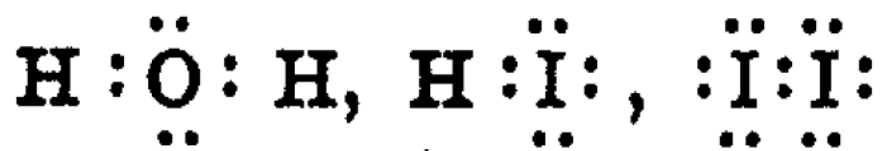


Figure 15: A) Gilbert N. Lewis (1875-1946); B) Dot notation for H₂O, HI, and I₂ from Lewis (1916).



Figure 16: Founders of *The American Mineralogist*: A) Samuel G. Gordon (1897-1952); B) Harry W. Trudell (1880-1964)

A

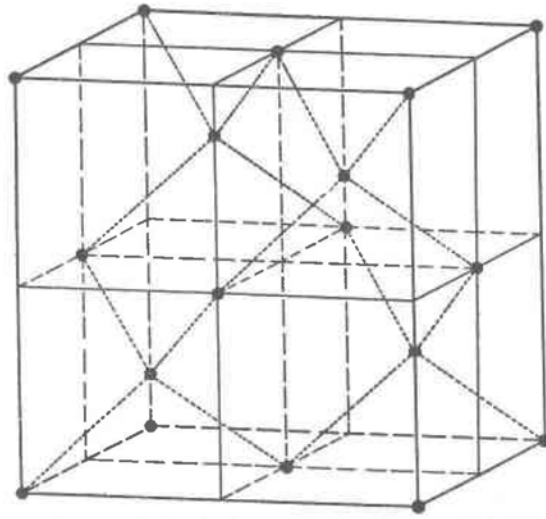


FIG. 1. Eight-atom cell of diamond lattice; valence of atoms 4, in directions shown by dotted lines.

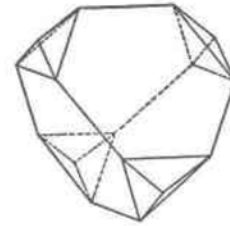


FIG. 2. Shape of each atom³ (when all are alike).

B

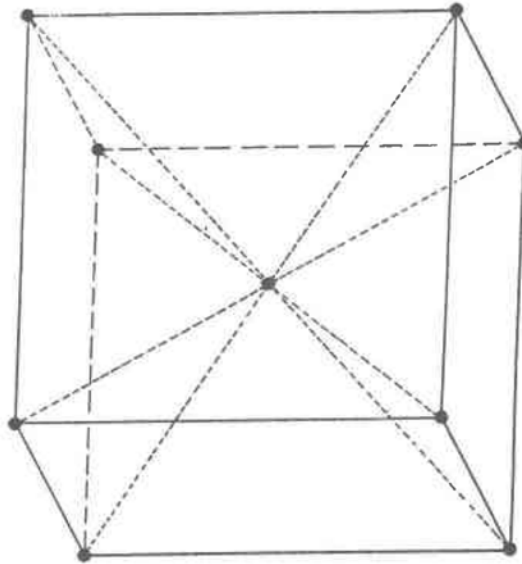


FIG. 5. Two-atom cell of body-centered cubic lattice; valence of atoms 8, in directions shown by dotted lines.

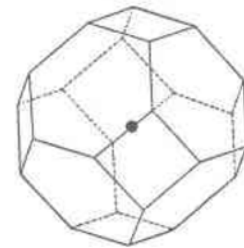


FIG. 6. Shape of each atom (when all are alike).

Figure 17: Wherry's (1918) representations of the structures of A) diamond and B)

body-centered cubic structures such as α -Fe. Note his inferred physical

shapes of the atoms required by the unit-cell geometries to the right.

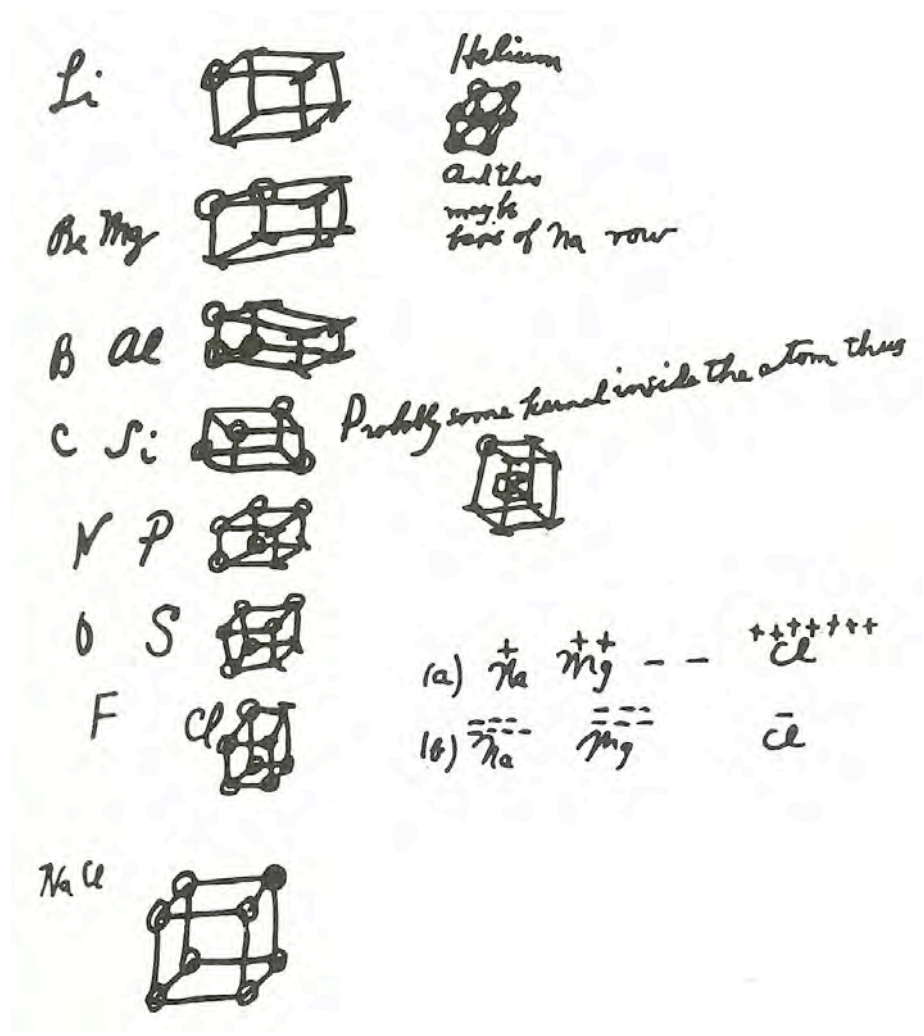


Figure 18: Lewis's sketches for the disposition of valence electrons around "cubical atoms," formalized in Lewis (1916).

Ann Arbor, Mich., February 5, 1917.

For several years past, some of those attending the annual meetings of the Geological Society of America have discussed the advisability of organizing a separate society composed of persons whose interests lie more especially in the field of Mineralogy. The feeling has been growing that the founding of a Mineralogical Society would do much to stimulate greater interest in the subject and also give wider recognition to the work being done in this field in America. Accordingly, the undersigned, who were in attendance upon the meetings of the Geological Society of America, at Albany, in December, 1916, discussed this question very thoroughly, and it was agreed that the time has come when an organization which might be called "The Mineralogical Society of America" should be formed at as early a date as possible.

While many of the advantages resulting from such an organization are apparent to all interested, the undersigned felt that perhaps the greatest benefit to be derived would be the founding by the society of a journal to be devoted exclusively to the publishing of mineralogical papers. As is well known, there is great need for a dignified medium of publication for the increasing volume of mineralogical investigations which are being carried on in America. Naturally such a publication must be started on a modest basis, and appear perhaps at first as a quarterly. Members of the society would of course receive the Journal free of charge.

With respect to organization and means of publication, mineralogists in America are far behind their colleagues in Europe, but we feel confident that you will respond promptly and favorably to our appeal to unite with us as a charter member in perfecting the organization of this society, the standards of which are to be on a par with those of the Geological Society of America. In order to insure the publication of a journal, which would naturally have a somewhat limited circulation, it was thought advisable that the annual dues be placed at \$10.00.

This letter is being addressed to a selected list of mineralogists in the United States and Canada, and if a sufficient number of favorable replies is received, it is planned to complete the organization sometime during the current year.

Professor Edward H. Kraus, Ann Arbor, Michigan, has been designated to conduct the correspondence looking toward the organization of the society. He will be glad to hear from you at your earliest convenience.

Very sincerely yours,

EDWARD H. KRAUS,	THOMAS L. WALKER,
ALEXANDER H. PHILLIPS,	EDGAR T. WHERRY,
FRANK R. VAN HORN,	HERBERT P. WHITLOCK.

Figure 19: The Founders' Letter circulated in 1917. [From MSA Centennial website]

CRYSTALLOGRAPHICAL AND MINERALOGICAL SOCIETY OF AMERICA

FOR several years the formation of a Crystallographical and Mineralogical Society of America has been contemplated, but the final steps leading to organization were postponed until after the close of the war. Those most concerned in the undertaking have recently been canvassed, and it is now expected that the society will be definitely organized during the meetings of the Geological Society of America in Boston, December 29 and 31.

Figure 20: The announcement in the Nov. 28, 1919 issue of *Science* of the founding of the "Crystallographical and Mineralogical Society of America."

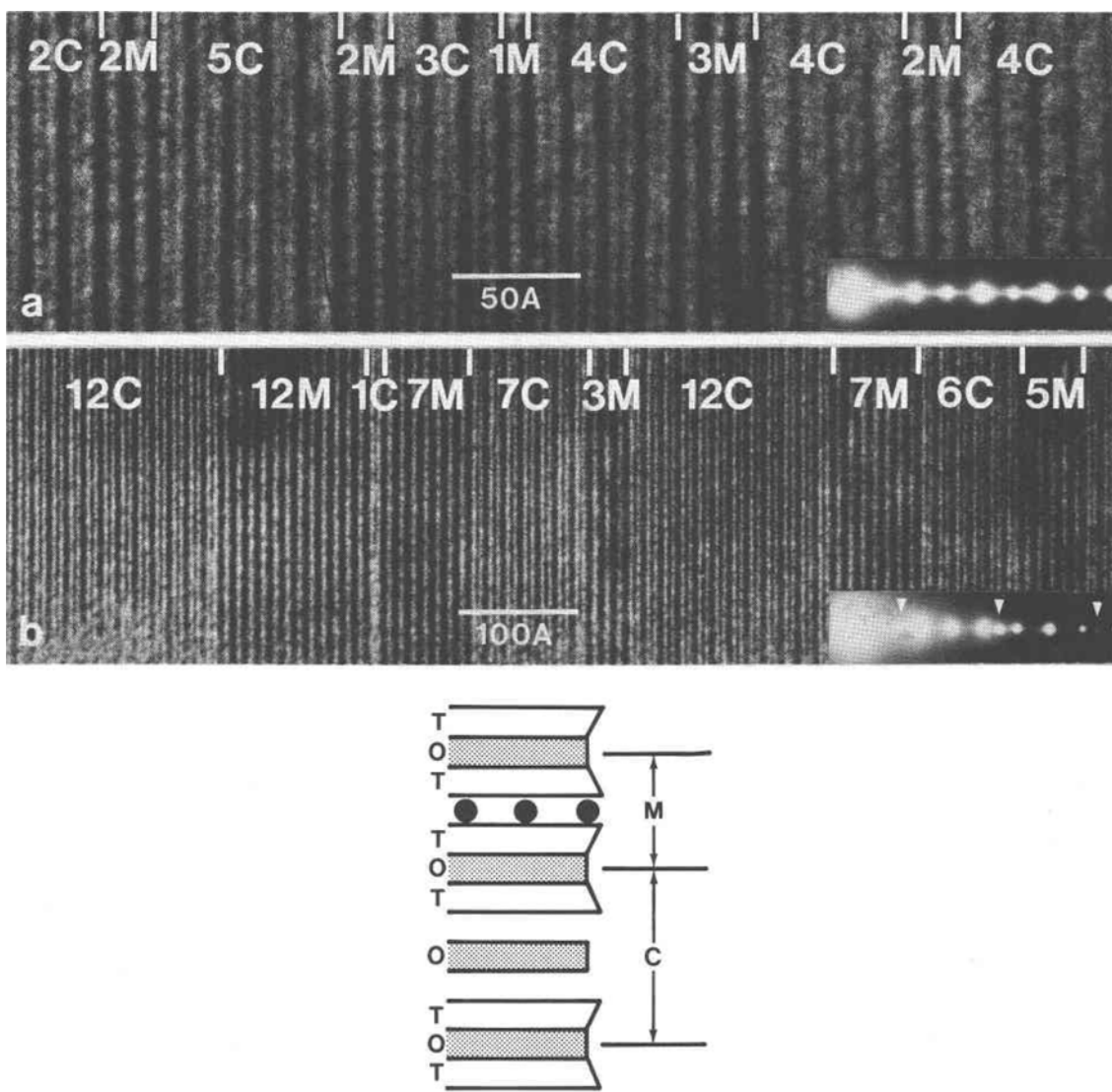


Figure 21: Fine (A) and coarse (B) slabs in mixed-layer chlorite (“C”)-mica (“M”) intergrowths with c^* horizontal. Inset diffraction patterns show heavy streaking along $00l$ due to the fine intergrowths. Diagram at bottom shows the structure of the nonconventional C (chlorite) and M (mica) slabs. Reprinted from Veblen (1983).

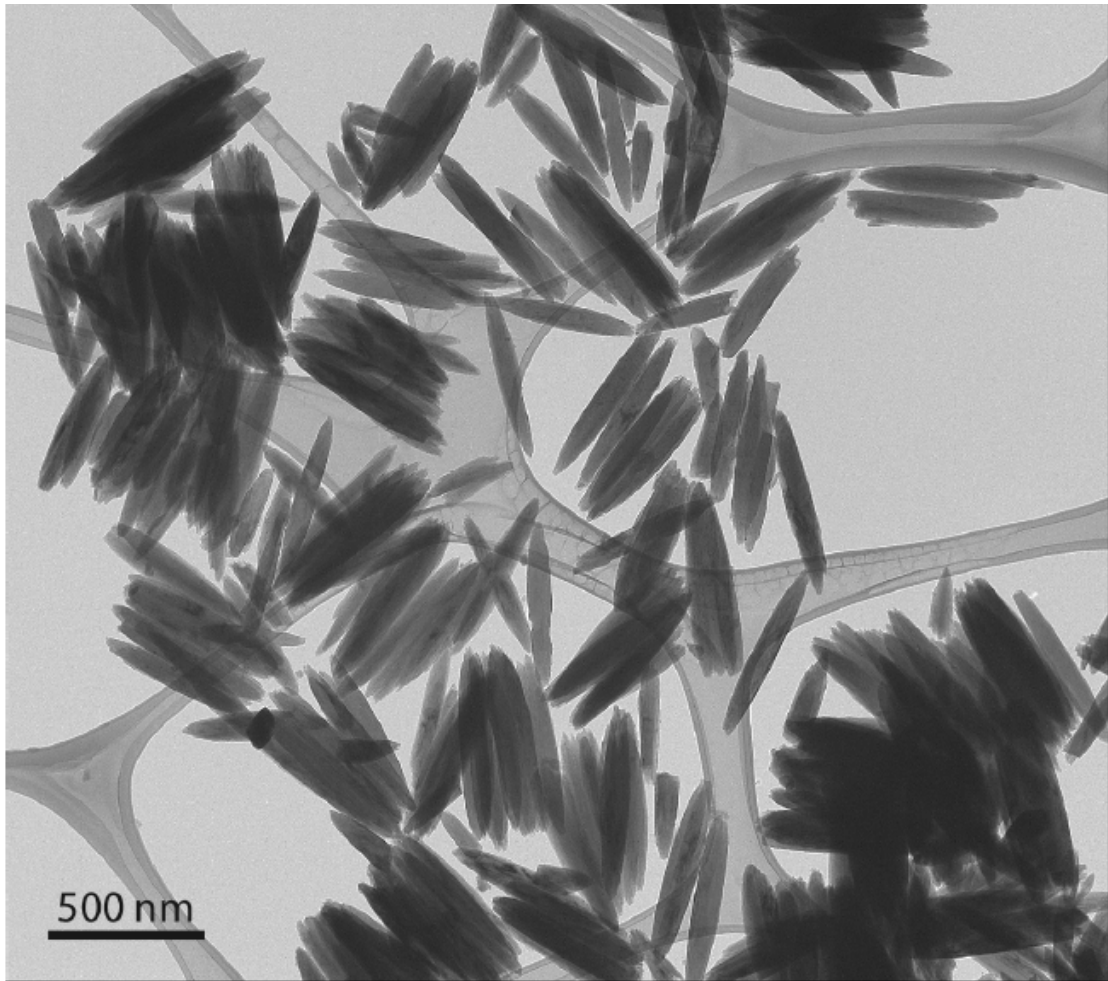


Figure 22: Transmission electron microscope images of synthetic akaganeite (γ -FeOOH) nanoparticles. Published with permission of Kris Peterson.