American Mineralogist, Volume 73, pages 670–672, 1988

Acceptance of the Roebling Medal of the Mineralogical Society of America for 1987

G. V. Gibbs
Department of Geological Sciences, Virginia Polytechnic Institute and State University, Blacksburg, Virginia 24061, U.S.A.

Mr. President, Professor Bloss, Honored Guests, and Fellows and Members of the Mineralogical Society of America:

When my colleague Paul Ribbe informed me at last year's GSA meeting that I had been selected as this year's Roebling Medalist for my work in mineralogy, I was surprised and a bit lost for words. I had not expected such an award, but I must admit that I am both pleased and honored that the society has seen fit to recognize me in this way. But, my work in mineralogy was not done alone. It was done in collaboration with a number of mineralogists, geochemists, chemists, physicists, and mathematicians. I owe a great debt to these talented and bright people for having taught me so much and for having shared with me their insights, knowledge, and ideas. Indeed, it was the instruction and help provided by these people and by my students and teachers that made the award possible.

I also owe a great debt to the U.S. Congress for enacting the GI Bill, legislation that made it possible for me to finish high school after a four-year hitch in the U.S. Navy and to attend college. I also owe a geat debt to my M.S. and Ph.D. advisors, Don Bloss and Joe Smith, two brilliant scientists, who saw to it that I learned that "There is nothing more practical than theory" and that I obtained training in mathematics, chemistry, and physics as well as in mineralogy. Clearly, meaningful research in mineralogy cannot be done today without a good background in these disciplines. Last, but by no means the least, I owe my greatest debt to my beautiful wife Nancy whose love and support have made my life a very happy and fulfilling experience.

Now for a little history of my experiences as a mineralogist. My interest in minerals and mineralogy began as an undergraduate at The University of New Hampshire and continued as a graduate student at The University of Tennessee where I had the good fortune of working with my very dear friend Don Bloss on the cleavage properties of quartz. My training in mineralogy at UNH had been in hand-specimen mineralogy replete with borax beads, charcoal blocks, blow pipes, and hand lens. I received no training whatsoever in crystallography and crystal chemistry, but I sure could make a beautiful borax bead. Recognizing these deficiencies, Don urged me to study Bragg's classic book on the atomic structure of minerals. Not only did this book expose me to the wonders of the microscopic world of minerals, but it also exposed me for the first time to the exciting papers and ideas of Linus Pauling, V. M. Goldschmidt, and W. H. Zachariasen. Upon completing my M.S. degree and working summers at the U.S. Bureau of Mines at Norris, Tennessee, where I discovered protoamphibole, I followed Don's advice and applied to and was accepted by the Graduate School at The Pennsylvania State University to work with Joe Smith on amphiboles. I could not have made a better choice of universities to undertake an advanced degree in mineralogy and geochemistry nor of advisors to work under.

Following a thesis defense on a crystal-structure determination of protoamphibole, an exciting and rewarding post-doc at The University of Chicago working with Joe Smith on forsterite and pyrope, and a year at Union Carbide working with Don Breck and Edith Flanigan on zeolites and emerald laser crystals, I returned to Penn State as an assistant professor. It was here that I had the good fortune of meeting Gordon Brown, Pat Meagher, and Gary Novak, the first of more than 20 very bright and gifted graduate students whom I have had the privilege of working with over the years. Pat and I undertook the task of unraveling the polymorphism of cordierite and found that it resembled that of K-feldspar in many ways. But, before Gordon and I could get started on a problem, I was offered a position at Virginia Tech where Byron Cooper had the vision of establishing a center of mineralogical research. What made the offer so exciting was that he had also made similar offers to Paul Ribbe and Don Bloss with the proposal that all three of us come to Tech as a team. My decision to accept Byron's offer left Gordon with the difficult choice of either remaining at Penn State in a department of considerable reputation or coming with me to Virginia Tech.

It was my good fortune that Gordon elected to come to Virginia Tech. For his Ph.D. thesis, Gordon undertook a crystal-chemical study of the olivines. Meanwhile, Paul and I embarked on a similar study of the humites, Gary Novak took on a study of the garnets, and Maryellen Cameron, Judson Mitchell, and Keith Robinson began studies of the amphiboles. It was my belief that precise structural analyses on selected members of these mineral groups would not only improve our understanding of their crystal chemistry, but they would also provide valuable insight into the nature of the SiO bond. I thought, for example, that when a Mg atom in minerals like olivine and garnet was replaced by a more electronegative atom like Fe, electron density would be drained away from the oxygen atom in forming a more covalent bond, thereby weakening and lengthening the SiO bond. However, much to my surprise, we found that the SiO bond lengths in these minerals were largely unaffected by such substituents. In an attempt to find an explanation of this result, Gordon Brown and I set to reading the literature.

Meanwhile, NSF had generously awarded our department a Centers of Excellence Grant that had funds for inviting Durward Cruickshank as a visiting distinguished professor of geochemistry and John Louisnathan as a research associate to Virginia Tech. What followed was a very exciting time for me. Gordon and I wrote several papers unrelated to his thesis work in which we attempted to rationalize the stereochemistry and Al-Si ordering patterns of aluminosilicates in terms of Cruickshank's bonding model. It was also during this time that we discovered a very important paper by J. C. Slater in which he resurrected Bragg's atomic radii and showed that a single set of radii could be used to reproduce bond lengths in molecules and crystals alike, regardless of bond type. It was then that we began to suspect that the forces that govern bond-length and bond-angle variations in a crystal were not unlike those in a chemically similar molecule. If true, then it occurred to us that perhaps molecular orbital calculations on a silicate molecule might provide an explanation of some of the empirical correlations that had been established for the silicates between SiO bond length, SiOSi and OSiO angle, and bond-strength sum.

At this time in my career I knew little about molecular orbital theory and how it might be used to provide insight into the force field that governs the structure of a silicate molecule. However, in reviewing the literature, I ran across a paper by Larry Bartell, a brilliant chemist at The University of Michigan, who had used bond-overlap populations obtained with semiempirical molecular orbital theory to rank the observed bond lengths in phosphate and sulfate molecules. I wrote Larry a letter explaining to him that I knew little about the theory, but that I thought that it might prove useful in providing a qualitative understanding of bond-length and bond-angle variations in silicates. To make a long story short, Larry was more than eager to work with me in applying the method to silicates. Not only am I grateful to him for tutoring me in the theory, but more important, for carefully instructing me in its strengths and weaknesses.

Using what I had learned, calculations were completed in collaboration with students and colleagues alike on a variety of minerals and inorganic compounds ranging from borates to selenates. Although these calculations provided a connection between bond-length and bond-angle variations, they were too crude to make quantitative predictions. Following this work, I had the good fortune of meeting Mike O'Keeffe, Marshall Newton, and Jack Tossell, three very gifted chemists who patiently instructed me in the fundamentals of nonempirical computational chemistry and showed me how Born-Oppenheimer surfaces can be used to provide an explanation of bond-length and bond-angle variations, bulk moduli, and vibrational spectra of silicate molecules and crystals. It was also during this time that I met my very good friend Monte Boisen, a brilliant algebraist to whom I owe a great debt for teaching me the fundamentals and beauty of group theory and linear algebra. My collaboration with him not only improved my understanding of mathematics, but, among other things, it has also taught me the importance of the equivalence relation and conjugacy classes in the study of crystallography. Not only have Monte and I collaborated extensively in the last few years in the study of mathematical crystallography, but also in the mathematical modeling of the structures and elastic properties of crystals and molecules.

I also owe a debt to Bob Stewart and Mark Spackman, two brilliant chemical physicists at Carnegie Mellon University, for selflessly helping Jim Downs, Rod Hill, Karen Geisinger, and me undertake multipole analyses of the electron-density distributions in coesite, stishovite, phenacite, and bromellite. I also have fond memories of visiting my very good friend Pat Meagher at The University of British Columbia, of the excitement of generating the first-energy surfaces for such molecules as disilicic acid, and of Larry Finger's exciting visit to Tech in 1982 when we found that theoretical electron-density maps calculated for a disilicic acid molecule yield bonded radii for Si and O that matched those observed for the silica polymorphs. I also wish to thank Alex Navrotsky, a lady of unusual intellect, for showing me how our molecular orbital calculations can be used to interpret the thermodynamic properties of crystals, glasses, and melts; Mark Bukowinski, a brilliant geophysicist, for patiently teaching me the fundamentals of elasticity theory and its use in obtaining an equation of state; Jeremy Burdett, a gifted and articulate chemist, for showing me the role that angular overlap plays in determining molecular and solid state geometry; and my very talented and bright students

Kurt Bartelmehs, Bryan Chakoumakos, Philippe D'Arco, Bob Downs, Jim Downs, Karen Geisinger, Dana Griffen, George Lager, Curtis Lindsay, Ron Peterson, and John Schlenker for sharing with me their ideas on the meaning and significance of our many calculations and their relation to the real world. Finally, I also owe a debt to another brilliant friend of mine, Tony Lasaga, who showed me how the methods of crystal molecular mechanics can be used to generate the structures, the equation of state, and lattice dynamics of the silica polymorphs and how MO-derived activation energies and vibrational frequencies can be used to compute partition functions for evaluating the rate constants of geologically important molecular reactions.

In closing, I must thank Paul Ribbe for many years of fruitful and exciting collaboration and Don Bloss for his valuable council over the years. For me, it is a privilege and great source of pleasure that Don gave my presentation address and that Paul, the president of our society, made the award. Thank you.