American Mineralogist, Volume 88, pages 1–10, 2003

A molecular dynamics study of the behavior of sodium in low albite

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ABSTRACT

The structural features of albite (atomic coordinates and distances, thermal displacements) at 25 and 1040 °C, obtained by Molecular Dynamic simulations following the Car-Parrinello approach, were favorably compared with those obtained by single-crystal diffraction experiments. Starting from this basis, it was shown that the marked anisotropy of electron density distribution about the positions of the sodium atoms is due to a time average of highly anisotropic thermal vibrations, and not to a space average of multiple positions occupied by Na. Although the large displacement of Na from its center of gravity results in great variations over time of the individual Na-O distances of the sodium coordination polyhedron, the average distance remains approximately constant, reaching its minimum variation when the 9 nearest O atoms are considered, thus supporting a true 9-coordination of sodium.