Compressibility mechanisms of alkali feldspars: New data from reedmergnerite

R.T. Downs,* H. Yang, R.M. Hazen, L.W. Finger, and C.T. Prewitt

Geophysical Laboratory, Carnegie Institution of Washington, 5251 Broad Branch Road, N.W., Washington, D.C. 20015, U.S.A.

ABSTRACT

Structural and volume compressibility data for reedmergnerite, NaBSi$_3$O$_8$, were obtained by single-crystal X-ray diffraction at pressures up to 4.7 GPa. The bulk modulus was determined to be 69.8(5) GPa with the pressure derivative constrained to 4. Unit-cell compression is anisotropic, as indicated by unit strain tensors. Tetrahedral bond lengths and angles remained relatively constant over the pressure interval, whereas Na-O bonds decreased systematically. T-O-T angles underwent a variety of behaviors, remaining constant or decreasing with pressure.

The compression for reedmergnerite is similar to that of low-albite, wherein bending of the (Al,B)-Oco-Si angle compresses the Na-bearing zigzag channels. In contrast, microcline compresses by shearing the four-membered rings, which in turn compresses the K-bearing channels. At about 4 GPa, a new bond between K and Obm appears that alters the compression mechanism and explains the discontinuity in the pressure variation of crystallographic parameters observed by Allan and Angel (1997). Thus, the compression mechanism of the alkali feldspars is dominated by the compression of alkali containing channels. However, because of low symmetry, this can be accomplished in several ways. The observed variety of compression pathways resulted from T-O-T angle bending energetics that were coupled with the effects of alkali cation bonding.

INTRODUCTION

Feldspars are crustal materials and therefore not naturally subjected to high pressure. However, considerable interest exists in the response of the feldspar structure to pressure. For example, such low-density structures exhibit both subtle and extreme structural changes when subjected to only modest pressures and, furthermore, the low symmetry of ordered feldspars maximizes the degrees of freedom associated with compression mechanisms.

Compression mechanisms are structurally controlled. Whereas highly symmetric closest-packed deep earth materials compress mainly by bond shortening, shallow earth materials mainly compress by bond angle bending. For example, Si-O-Si angle bending correlates with the compressibility of the SiO$_2$ polymorphs (Hemley et al. 1994). They all seem to fall on the same $\Delta V - \Delta(Si-O-Si)$ trend (Downs and Palmer 1994). The compressibility of an individual silica structure is simply related to the displacements of the $\langle Si-O-Si \rangle_0$ angles from their global equilibrium value ($\sim 144^\circ$); the further from equilibrium, the stiffer the structure. However, the feldspars are not as simple. The T-O-T angle differs from being only Si-O-Si, as in silica, to being a mix of, for instance, Si-O-Si and Al-O-Si (or B-O-Si). These angles have significantly different curvatures in their variations with energy. Al-O-Si appears to be twice as soft as Si-O-Si, whereas B-O-Si is twice as stiff (Nicholas et al. 1992). If compressibility of feldspars was dependent only upon these factors, then albite, potassium feldspar, and anorthite should be softer than the low-density silica polymorphs because the Al-O-Si angle is weaker than the Si-O-Si angle. Instead, the feldspars are generally stiffer; bulk moduli for quartz, cristobalite, and the high-pressure polymorph, coesite, are 37, 11, and 100 GPa, respectively (Angel et al. 1997; Hemley et al. 1994) but equal 55, 60, 80, and 69 GPa for albite, microcline, anorthite, and reedmergnerite, respectively (Angel 1994). Thus, the M-cation must effect compressibility, even though compression proceeds through T-O-T angle bending.

The M-cation affects the bending energy of the T-O-T angle primarily through the charge of the M-cation and the M-O bond length. Also, the energy required for the bending of a T-O-T angle is significantly increased if the bridging O is bonded to three or more atoms (Geisinger et al. 1985). An atom with more electrons to contribute to bonding will produce a stronger bond than another atom with fewer electrons at the same bond length, and as the bond lengthens, the electron density becomes more diffuse and, therefore, the contribution to the bonding energy is lower. These effects are demonstrated by comparing the compressibility of anorthite (Angel 1994) containing Ca with feldspars containing Na or K. If compression were controlled only by the T-O-T angles, then anorthite, with every bridging angle between Al and Si, should be more compressible than sodium or potas-