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An alternative method of calculating cleavage energy: The effect of compositional domains in micas

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Abstract

Cell parameters and atomic coordinates for the true micas are varied to simulate layer deformation along the [001]* direction by an external force. The resulting (deformed) structures are then used to determine bonding forces and to calculate a maximum force component along the [001]*. Bonding forces are compared to experimental observations of bond lengths of the interlayer, octahedral, and tetrahedral sites. Calculated bonding forces are consistent with experimental observations that locate the cleavage plane along the interlayer. Because many studies have shown that the chemical composition of the cleavage surface often differs from the structure of the bulk, compositional variations were considered in determining cleavage energy. The chemical composition of the cleavage surface may produce a reduction in cleavage energy. This reduction in energy depends on various elements occurring in greater number at the cleavage surface than in the bulk. A reduction in cleavage energy occurs if there is a reduction in the interlayer site size, as measured by the area defined by the first-coordination basal oxygen atoms. In addition, a reduction in lateral cell dimensions and an increase in the bonding force between the basal oxygen atoms and the interlayer cation also results in a reduction in cleavage energy in the direction normal to the layer.

Joins considered are phlogopite–annite, tetra-ferriphlogopite–tetra-ferri-annite, polylithionite–siderophyllite, muscovite–celadonite, and muscovite–paragonite. A lack of homogeneity in composition may produce preferential cleavage locations within the family of (001) planes. The cleavage energy appears to be greater for homogeneous synthetic micas compared to natural micas.

Keywords: Micas, cleavage, electrostatic force, crystal chemistry, crystal structure