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Influence of crystal chemistry on ideal plastic shear anisotropy in forsterite: First principle calculations

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ABSTRACT

We present ab initio calculations of ideal shear strengths (ISS) in forsterite at zero temperature using pseudopotential density functional theory within the generalized gradient approximation. A localized rigid-body shear is imposed on a given plane of an infinite defect-free crystal. The energy increase associated with this shear (called the generalized stacking fault energy) gives access to the ISS. The goal of this study is to assess the influence of crystal chemistry on the intrinsic resistance of plastic shear of a mineral like forsterite. ISS have been calculated for plastic shear along [100], [010], and [001] in various potential glide planes of forsterite. We show that the [001] slip, which corresponds experimentally to an easy glide at low temperature, exhibits the lowest energy barrier. The [010] glide is precluded because it involves very unfavorable atom impingements.