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# Dislocation modeling in calcium silicate perovskite based on the Peierls-Nabarro model

**Denise Ferré, Patrick Cordier,* and Philippe Carrez**

Laboratoire de Structure et Propriétés de l'Etat Solide, UMR CNRS 8008, Université des Sciences et Technologies de Lille, 59655 Villeneuve d'Ascq Cedex, France

## Abstract

In this study, we propose a study of dislocations and plasticity in $CaSiO_3$ perovskite based on the Peierls-Nabarro modeling using the generalized stacking fault (GSF) results as a starting model. The GSF are determined from first-principle calculations using the VASP code. The dislocation properties such as planar core spreading and Peierls stresses are determined for the four possible slip systems: $\langle 110\rangle\{1\bar{1}0\}$, $\langle 100\rangle\{011\}$, $\langle 110\rangle\{001\}$, and $\langle 100\rangle\{001\}$ and at 0, 30, and 100 GPa. We find that $\langle 110\rangle\{1\bar{1}0\}$ is the easiest slip system, but more surprisingly, we show that it bears no Peierls friction, even at the higher pressure. The reasons lie in the ability of these dislocations to split into partial dislocations and in the nature of the stacking fault associated with it.

**Keywords:** $CaSiO_3$ perovskite, deformation mechanisms, dislocations, slip systems, first-principle calculations, DFT, Peierls-Nabarro model