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Dislocation core modelling in diopside with the Peierls-Nabarro model

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Clinopyroxenes are important constituents of the upper mantle in a pyrolitic model. These minerals present a strong elastic anisotropy which, combined with crystal preferred orientations (CPO) due to the plastic deformation, could contribute to the seismic anisotropy of the upper mantle. The CPOs are developed by an anisotropic mechanism of plasticity, such as dislocation creep where dislocation mobility is governed by the core structure of the defect.

In this work, we calculate the dislocation properties of $CaMgSi_2O_6$diopside, the magnesian end-member of clinopyroxenes, at 0GPa and 10GPa using the Peierls-Nabarro (PN) model. The so-called PN model is a fundamental concept of the dislocation theory which describes the resistance of the lattice to dislocation motion, a very important factor for the plasticity of silicates. The PN model also provides an analytical description of the dislocation core and of its potential spreading in the glide plane. Known for several decades, the PN model has triggered a renewed interest when Christian and Vitek (1970) showed that realistic models of dislocations could be built by incorporating generalized stacking faults (GSF) into the PN model. Here, we use a parameterized potential and the GULP code to calculate the GSFs which are incorporated in the PN model. In that way, we obtain a model of the dislocation core profile and the value of the stress required to move a dislocation (the so-called Peierls stress) for six slip systems in diopside.

We show that the 1/2<110>{110} and the [001]{110} dislocations present low Peierls stresses as well as 0 and 10GPa. The [001](100) slip system has a complex dislocation core structure and a similar lattice friction as the [001]{110} slip system. Finally, we propose complex sessile dislocation core structures for the [100](010) and [010](100) dislocations which could be explain the difficulties to activate these slip systems experimentally.