Sulfur Impurities in Zirconium: Ab-Initio Study in the Bulk and in Screw Dislocations

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Sulfur impurities were shown recently to have a dramatic effect on the mechanical properties of hcp-Zr: 25 ppm of sulfur are sufficient to reduce the creep rate by a factor of 3. Since few experimental data are available in the Zr-S system, we have investigated the behavior of sulfur impurities in hcp-Zr using DFT-LDA pseudopotential calculations, both in the bulk and in a screw dislocation.

By comparing the energies of various interstitial configurations and of the substitutional configuration, sulfur is shown to dissolve preferentially in octahedral sites. The expansion of the octahedron volume is intermediate between that for an oxygen impurity and for a self-interstitial. The calculated activation energy for sulfur diffusion in zirconium is in good agreement with experiments. Calculations performed in a screw dislocation indicate that S tends to segregate at the core of the dislocation and that it induces a strong modification to dislocation core structure. This result supports the mechanism proposed to explain the hardening effect of sulfur observed experimentally in zirconium.