Structural and electronic properties of Sigma-7 grain boundaries in alpha-alumina

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Applying simulated annealing with a classical potential followed by screening of low-energy structures with density functional theory, we examined the atomic and electronic structures of two Sigma-7 symmetric tilt grain boundaries in alpha-Al$_2$O$_3$. The lowest energy boundary of the two exhibits a pronounced pattern of alternating columns of exclusively four- or fivefold coordinated Al atoms, with a grain boundary energy of 1.84 Jm$^{-2}$. For the other boundary, numerous structures were found with energy just below 2.11 Jm$^{-2}$. Furthermore, by analysing the full set of candidate structures generated by simulated annealing for the two grain boundaries, we find that the number of fivefold coordinated Al atoms tends to increase with grain boundary energy, which we can also correlate with the behaviour of the electronic density of states. On the other hand, we find no systematic trend with energy that might be expected for other quantities, notably the excess volume of the interface.

We compare simulated high-resolution transmission electron microscope (HRTEM) images of the lowest energy calculated structures with experimental images. The disparate structural and electronic features of these two boundaries suggest reasons for their very different oxygen diffusion coefficients that have been observed experimentally.