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First-principles calculation of impurity diffusion barriers in Al
NILS SANDBERG, RANDI HOLMESTAD, Dept. of Physics, Norwegian University of Science and Technology (NTNU), 7491 Trondheim, Norway — We have performed extensive electronic structure calculations to obtain impurity+vacancy formation energies, $H_{\rm iv}$, and impurity migration energies, $H_{\rm im}$, in Al matrix. The impurities considered are Mg, Si and the 3d transition metals (Sc-Zn). We have also estimated the correlation factor f, accounting for the 'non-randomness' of successive impurity migration jumps. The total effective impurity diffusion barriers $H_{\rm iD} = H_{\rm iv} + H_{\rm im} - {\rm d}\ln(f)/{\rm d}(1/k_{\rm B}T)$ compare well with experimentally measured diffusion barriers (see, e.g., evaluation in Du et al, Mater. Sci. Eng. A **363**, 140 (2003)). $H_{\rm iD}$ varies strongly over the 3d series transition metals, mainly due to a strong variation in the migration barrer $H_{\rm im}$, which explains why, e.g., Mn diffuses orders of magnitude slower than, e.g., Al (self diffusion). Mg, Si Zn and Cu are found to be fast diffusers compared to Al. Two main sources of error on the theory side are a) temperature dependencies in $H_{\rm iv}$ and $H_{\rm im}$ due to anharmonicity in the atomic vibrations and b) the choice of exchange-correlation approximation. Both these factors will be discussed.

Nils Sandberg
Dept. of Physics, Norwegian University of Science and Technology (NTNU)
7491 Trondheim, Norway

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