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DFT studies of the early stages of growth of Nb on MgO(100)[1]
YUNSIC SHIM, JACQUES G. AMAR, University of Toledo — Using DFT calculations of binding and adsorption energies for various sizes and shapes of Nb clusters on MgO(100) surfaces, we have examined the effects of cluster shape and a neutral O vacancy on the energies and stability of Nb[100] and [110] island structures. Similarly to other cases of metal adsorbates on MgO(100) surfaces, O-vacancy sites tend to act as nucleation sites for Nb adatoms, while the effect of a nearby O vacancy on the binding energy of a Nb cluster is much weaker. In particular, we find that the binding energy for a Nb monomer at an O site (O-vacancy site) is 1.52 eV (2.2 eV) while the energy barrier for Nb monomer diffusion is 0.58 eV. In addition, although both isolated 4-atom Nb [100] and 5-atom Nb [110] islands are isotropic with a slightly higher binding energy for the [100] island, for larger clusters an anisotropic Nb [110] structure is more stable than a square Nb [100] structure, which is in good agreement with a recent experimental result [1].

[1] M. Krishnan et al., Phys. Rev. ST. Accel. Beams 15, 032001 (2012).

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