Development of an embedded atom method potential for vanadium

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An embedded atom method (EAM) potential[1,2] for pure vanadium is being developed as the first step in the construction of an EAM potential for titanium-vanadium alloys. The potential is constructed using the force-matching method[3]: the functions comprising the potential are represented as cubic splines, and the spline knots are chosen such that the potential optimally reproduces a large database of forces, cohesive energies, and stresses computed via density functional theory (DFT). The code *potfit*[4] optimizes the splines using a combination of simulated annealing and conjugate gradient-like minimization algorithms. Preliminary EAM results are compared to DFT and experimental results for the lattice constant, cohesive energy, single-vacancy formation energy, fcc-bcc and hcp-bcc structural energy differences, elastic constants, and phonon dispersions.

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