Development and validation of neural network potentials for V–Ti–Cr alloys

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This work reports the development and validation of machine-learning interatomic potentials for the vanadium alloy V–4Ti–4Cr [1]. The training dataset was obtained from DFT (VASP) and includes Ti and Cr concentrations up to 15 at.% and high-temperature configurations. We show that configurations with anomalously short interatomic distances and large forces can destabilize fine-tuning of descriptor-based models; we also observed signs of non-physical behavior when using MatterSim for pretraining-based data generation. We fine-tuned and benchmarked NEP [2], DeepMD-DPA3 [3], and MACE potentials, obtaining comparable RMSE for energies, forces, and stresses, and then used a two-stage transfer learning workflow to train a fast DeePMD-SE potential for large-scale MD. Physical validation employed two-phase melting and stress–strain simulations at ambient pressure to estimate the melting temperature, Young's modulus, and Poisson's ratio; the results are consistent across potentials and agree reasonably with available experimental or literature data [4]. The work is supported by the Russian Science Foundation (project No. 25-29-01649).

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