Construction of interatomic potentials for multicomponent systems with stratified neural networks[1] SAMAD HAJINAZAR, ALEKSEY KOLMOGOROV, Binghamton University — Recent application of neural networks (NNs) to modeling interatomic interactions has shown the learning machines' encouragingly accurate performance for select elemental and multicomponent systems. In an effort to build extended libraries of NN-based models we have introduced a hierarchical training in which NNs for multicomponent systems are obtained by sequential fitting from the bottom up: first unaries, then binaries, and so on. Advantages of constructing NN sets with shared parameters include acceleration of the training process and intact description of the constituent systems. In the test case of the Cu-Pd-Ag ternary and its subsystems, NNs trained in the traditional and stratified fashions are found to have essentially identical accuracy for defect energies, phonon dispersions, formation energies, etc. The models' robustness is further illustrated via unconstrained evolutionary structure searches in which the NN is used for the local optimization of crystal unit cells. The use of NN instead of DFT in these simulations accelerates structure prediction by several orders of magnitude. The NN module is available in the MAISE package.

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