

Supplementary Material

In the supplementary materials, we have included detailed information regarding the training database in Section 1. We have provided a detailed analysis on the scalability of the MTP and DeePMD potentials as system sizes increase, which can be found in Section 2. Additionally, we have conducted evaluations to test the validity of the MTP and DeePMD potentials in systems with high concentrations of Nb, detailed in Section 3.

1 TRAINING DATABASE

We analyzed 28 initial structures for both γ -TiAl and α_2 -Ti₃Al, where some Ti atoms were substituted by Nb atoms to achieve the specified Nb concentration. Among these 28 configurations, a subset was set aside and not included in the training to evaluate the potential's predictive accuracy. Each of these structures (20 structures) underwent AIMD simulations in both the NVT and NPT ensembles at temperatures of 1 K, 300 K, 500 K, 700 K, and 900 K. Overall, we conducted 180 AIMD simulations: NVT simulations at 1 K, 300 K, 500 K, 700 K, and 900 K, and NPT simulations at 300 K, 500 K, 700 K, and 900 K. Snapshots from these AIMD simulations was treated as separate datasets, culminating in a total of 1,320,000 datasets. For the training and test sets, we carefully selected individual snapshots from the AIMD trajectories at specific intervals, thereby avoiding correlated data within our chosen datasets.

2 SCALABILITY OF POTENTIALS WITH SYSTEM SIZES

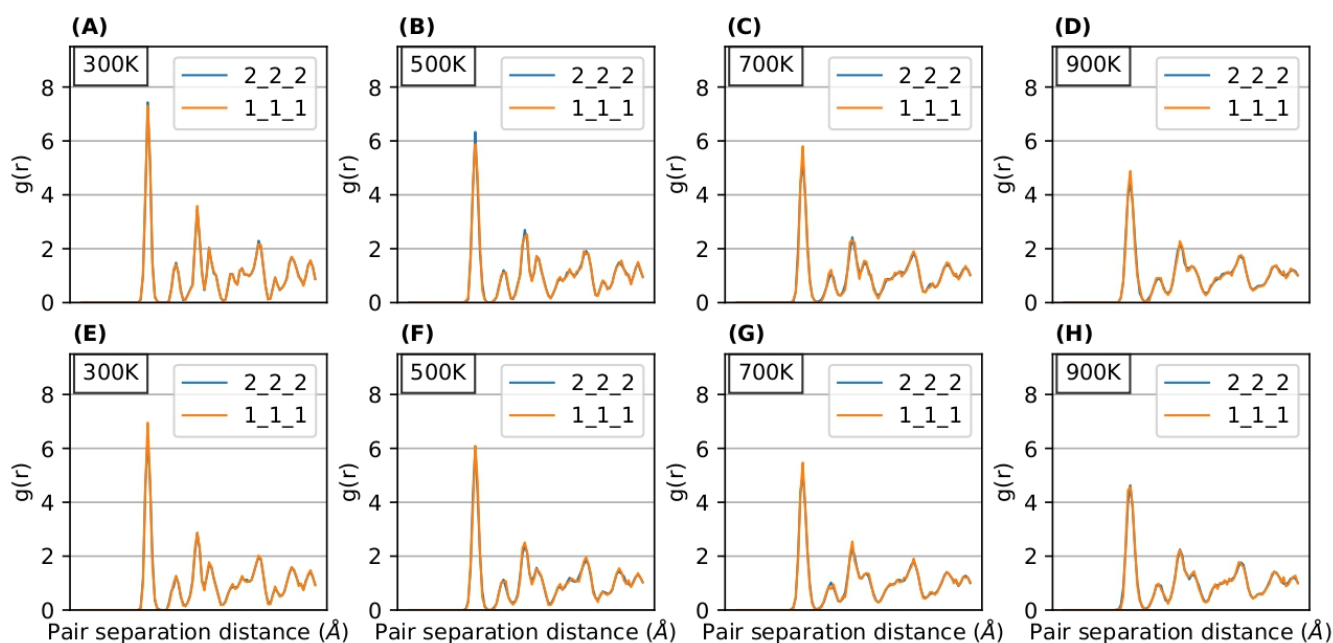


Figure S1. RDF curves for $2 \times 2 \times 2$ supercell and $1 \times 1 \times 1$ counterpart using DeePMD for α_2 -Ti₃Al. The top row (A-D) and the bottom row (E-H) correspond to the 2.3 at.% Nb and 6.3 at.% Nb models, respectively.

Here, we assess the scalability of the newly developed MTP and DeePMD potentials by varying the size of the system. Figures S3 and S1 display the RDF for the α_2 -Ti₃Al systems, comparing them with their

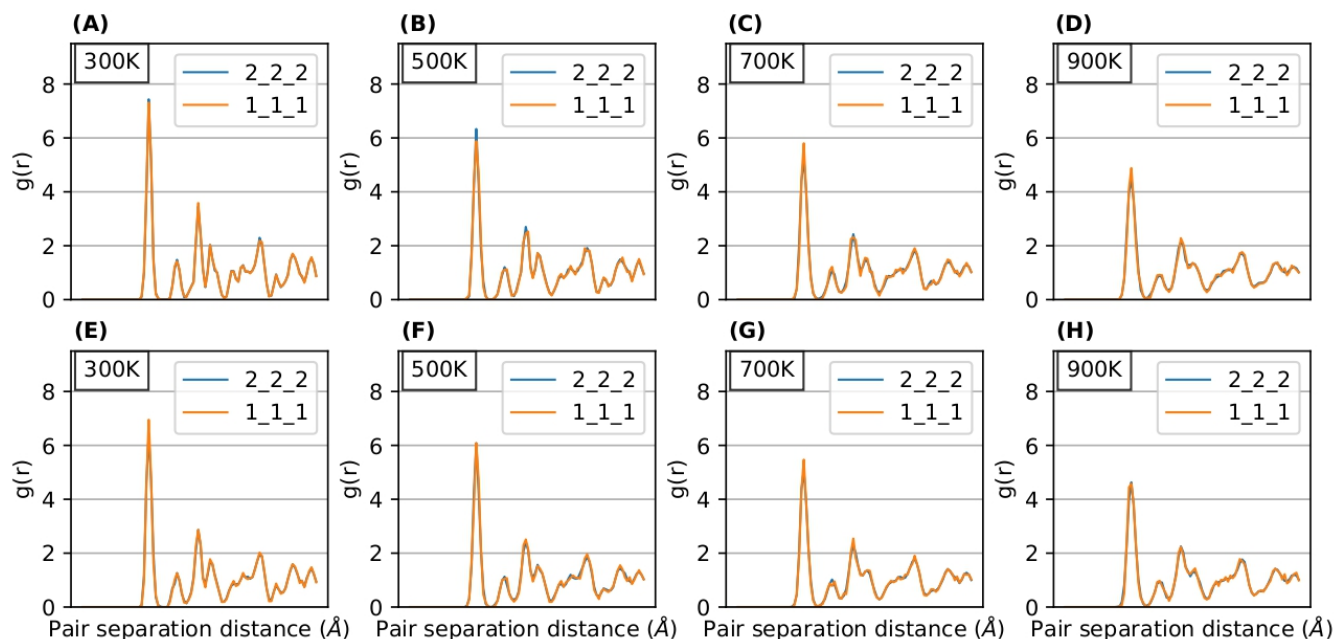


Figure S2. RDF curves for $2 \times 2 \times 2$ supercell and $1 \times 1 \times 1$ counterpart using DeePMD for γ -TiAl. The top row (A-D) and the bottom row (E-H) correspond to the 1.9 at.% Nb and 7.4 at.% Nb models, respectively.

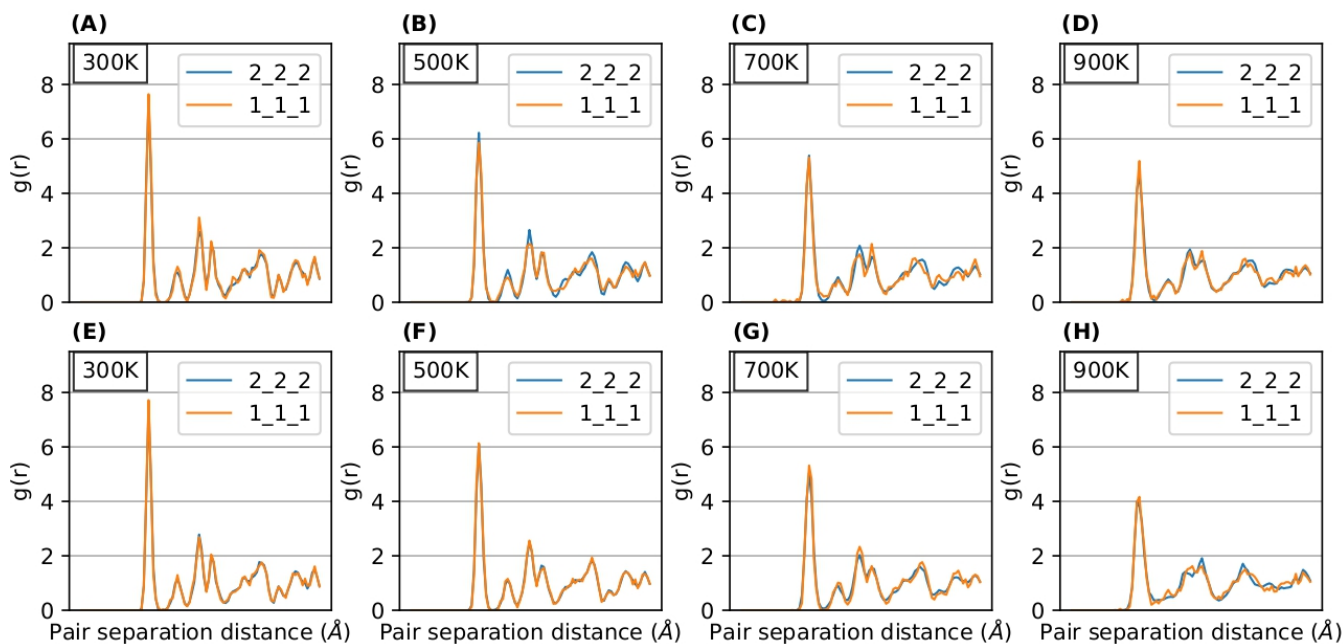


Figure S3. RDF curves for $2 \times 2 \times 2$ supercell and $1 \times 1 \times 1$ counterpart using MTP for α_2 -Ti₃Al. The top row (A-D) and the bottom row (E-H) correspond to the 2.3 at.% Nb and 6.3 at.% Nb models, respectively.

respective $2 \times 2 \times 2$ supercells containing 1024 atoms. Similarly, Figures S4 and S2 present the RDF for the γ -TiAl systems alongside their $2 \times 2 \times 2$ supercells containing 864 atoms. These figures demonstrate a good match between the RDF of the systems and that of their supercells, indicating that both MTP and DeePMD potentials exhibit effective scalability when the system size is increased.

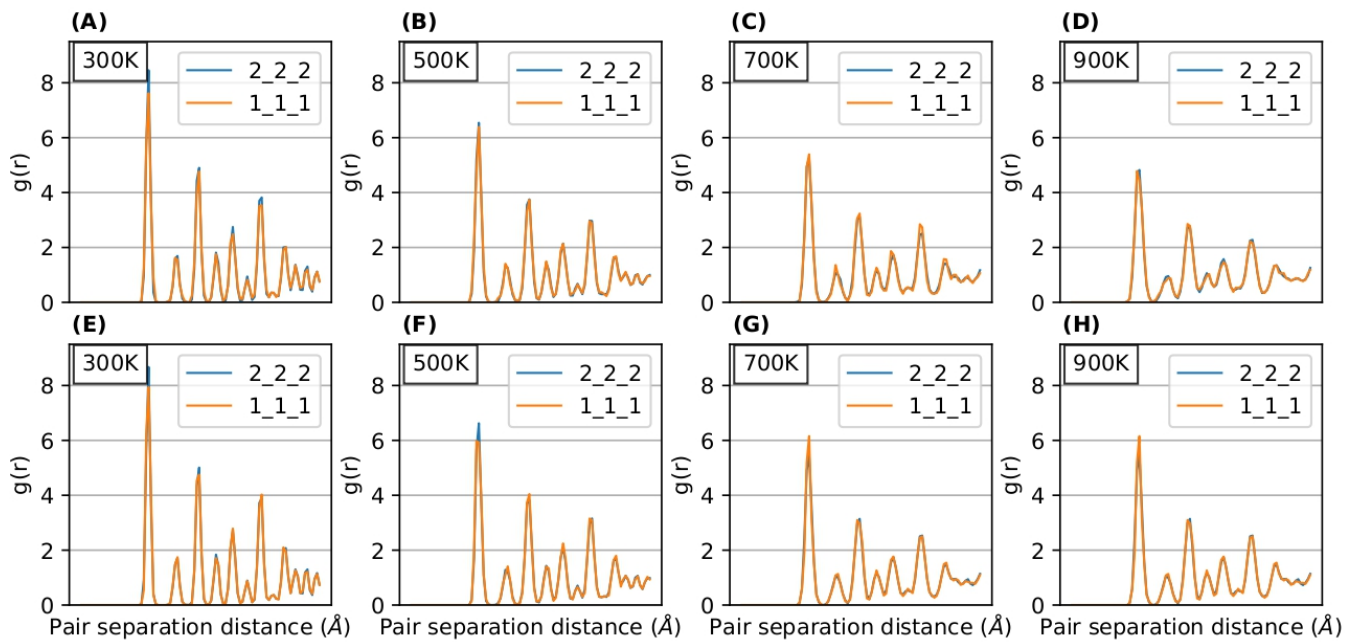


Figure S4. RDF curves for $2 \times 2 \times 2$ supercell and $1 \times 1 \times 1$ counterpart using MTP for γ -TiAl. The top row (A-D) and the bottom row (E-H) correspond to the 1.9 at.% Nb and 7.4 at.% Nb models, respectively.

3 TESTING THE VALIDITY OF POTENTIALS ON A SYSTEM WITH HIGH NB CONCENTRATION

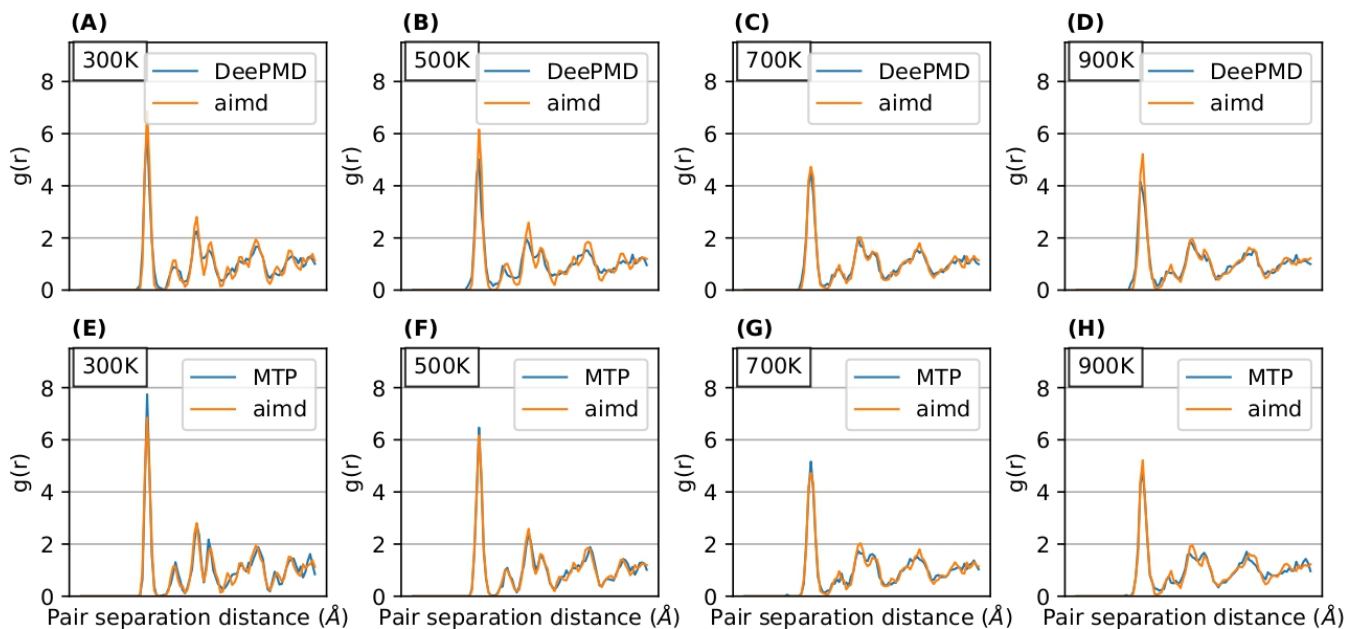


Figure S5. RDF curves of 14.8 at.% Nb concentration for α_2 -Ti₃Al using DeePMD (A-D) and MTP (E-H) potentials.

We also evaluated the validity of MTP and DeePMD potentials by testing them on a system with 14.8 at.% Nb concentration, which represents a higher Nb concentration than those included in the training

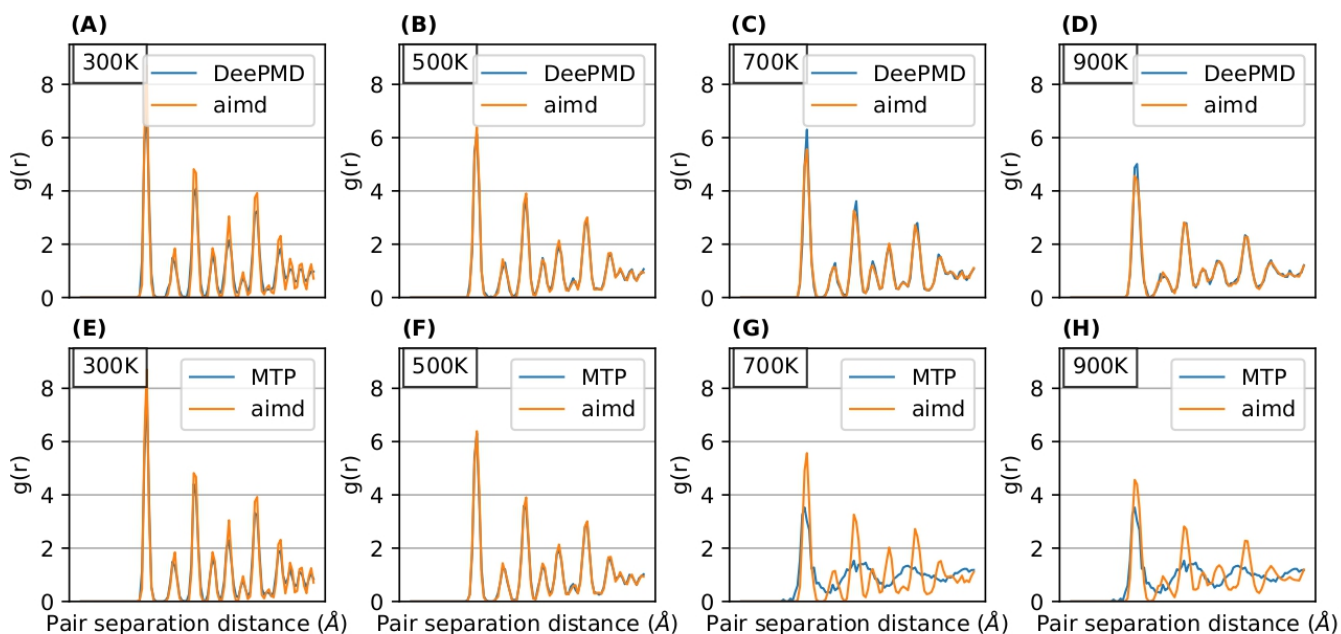


Figure S6. RDF curves of 14.8 at.% Nb concentration for γ -TiAl using DeePMD (A-D) and MTP (E-H) potentials.

datasets. Figures S5 and S6 compare the RDF of molecular dynamics (MD) simulations on models of α_2 -Ti₃Al and γ -TiAl with 14.8 at.% Nb concentration to those of AIMD simulations. The DeePMD potential demonstrated superior performance compared to MTP, showing a smaller deviation in RDF compared to that of AIMD. Specifically, in the case of MTP for γ -TiAl, the RDF exhibited a noticeable lack of agreement with that of AIMD, especially at higher temperatures (700 K and 900 K).