Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for "Molecular Dynamic Simulation of TC4 Titanium Alloy with Mechanical Property Calculations after Various Heat Treatment"

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Different from the hybrid treatment of binary EAM potential used in the manuscript, this file reports the results using ternary alloy potential TiAlV.eam.alloy generated from eam_database tool provided in LAMMPS. The EAM parameters for Ti and Al are obtained from study by Zhou et al.[1] while the EAM parameter for V are obtained from study by Zhao et al.[2]

1 Tensile Strength

1.1 Impact of Crystal Direction and Ensemble

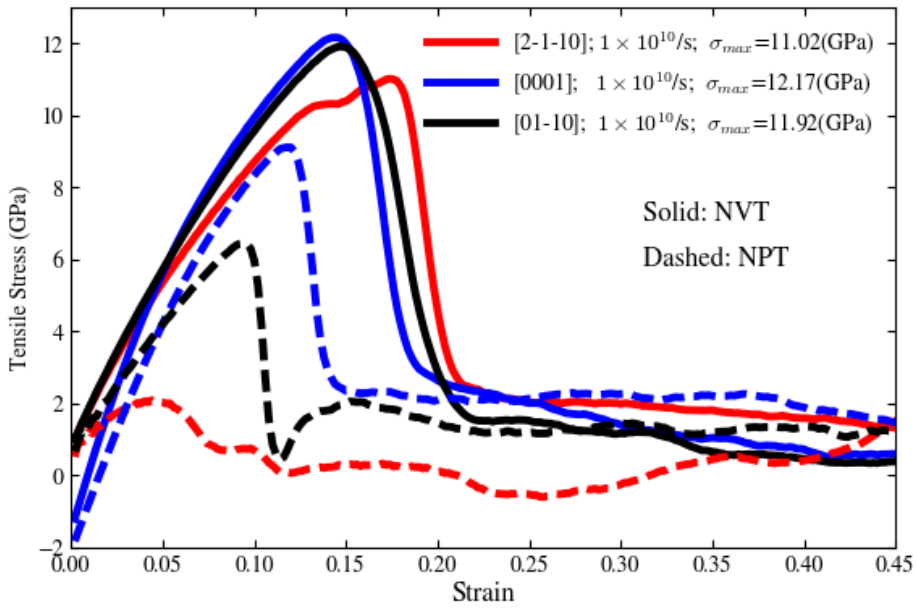

Fig. 1 For the 60x20x20 HCP model, stress–strain curves are compared between NVT (solid lines) and NPT (dashed lines) ensemble of tensile test along [2-1-10], [0001] and [01-10] directions respectively.

Similar to Figure 4 in the manuscript, the tensile strength is larger in [0001] direction than [2-1-10], and [01-10] directions as indicated by the comparison in Figure 1 above. At the same time, the tensile stress curves for NPT ensemble are

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consistently higher than NPT ensemble. The NPT ensemble differs from NVT ensemble in that zero pressure is applied along Y and Z axis, of which the dimension decreases with tensile deformation along X axis due to the Poisson's ratio effect. As a result, void and fracture is not observed in NPT ensemble under tensile loading as shown in the structural variations presented in Figure 2

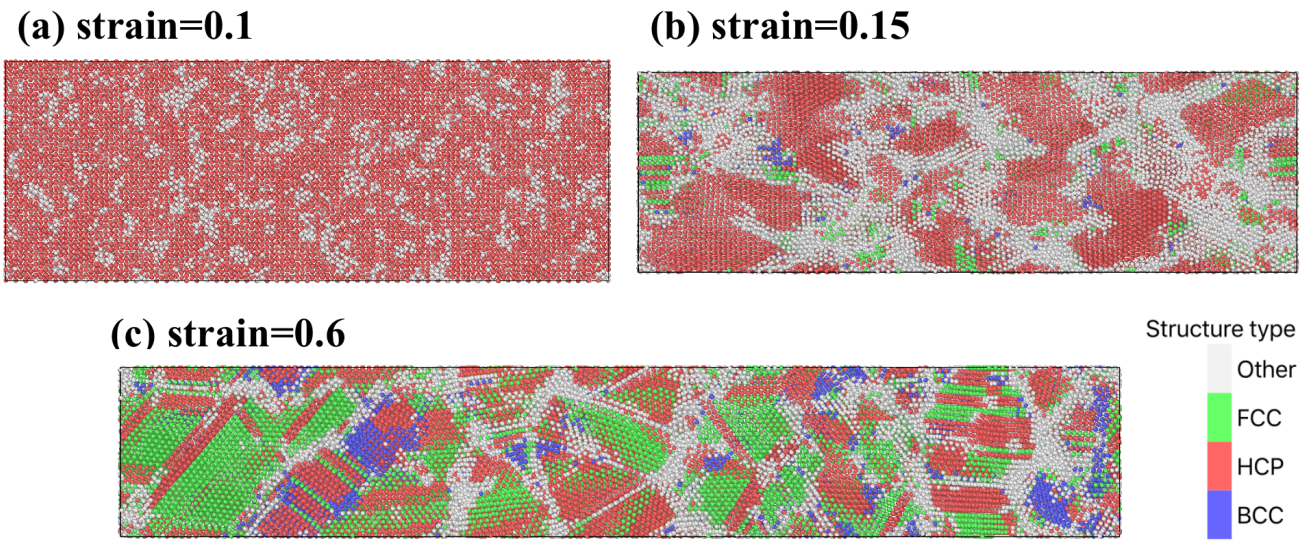

Fig. 2 The structural variation of 60x20x20 HCP model in NPT ensemble under tensile loading along [0001] direction at (a) strain=0.1, (b) strain=0.15 and (c) strain=0.6 respectively.

1.2 Impact of Heat Treatment

With EAM potential generated from eam_database tool, the impact of heat treatment becomes negligible as shown in details below. Firstly, the tensile strength without any heat treatment step already reaches 11.698GPa (red line in Figure 3), which is as high as the level after heat treatment in the manuscript. Secondly, neither annealing nor additional solid solution and aging improves the tensile strength when compared with no heat treatment. The nearly identical stress-strain curves in Figure 3) arises from the same HCP crystal structure, i.e. the 100% HCP fraction both before and after any heat treatment procedure. In contrast, the HCP fraction only rises from around 90% to 95% during the heat treatment process in Figure 6 of the manuscript. Thus, a stronger tendency to crystalize is observed by using the ternary EAM potential from eam_database than the hybrid treatment of binary EAM potential in the manuscript.

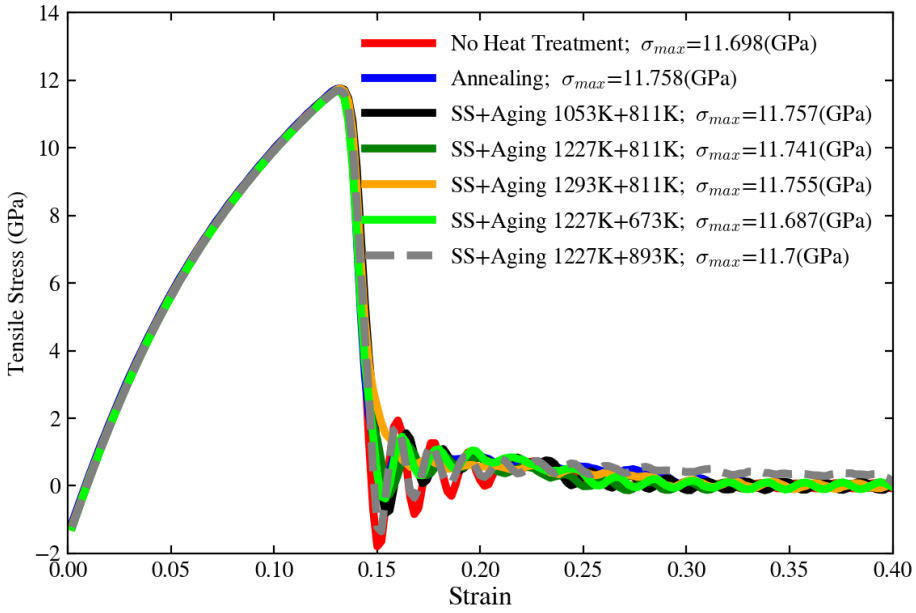

Fig. 3 Stress–strain curves for tensile test after various heat treatment procedures, with uniaxial tensile loading along [0001] direction.

2 Shear Strength

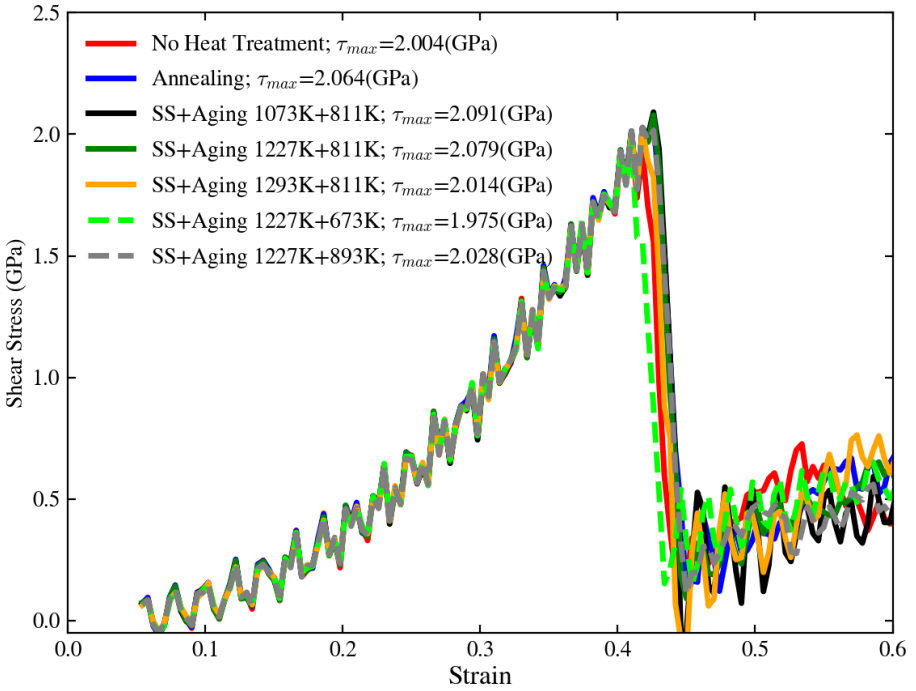

Fig. 4 Stress–strain curves for shear test after various heat treatment procedures.

Similar to tensile strength, the heat treatment's impact on shear strength is negligible with the ternary EAM potential. Figure 4 shows that additional solid solution and aging step slightly improves the shear strength, with largest shear strength of 2.091GPa obtained with solid solution at 1073K and then aging at 811K. Instead of the slipping of planes in Figure 9 of the manuscript, twin crystals in HCP region are observed in Figure 5(d) below, which can reduce the stress caused by phase transformation.

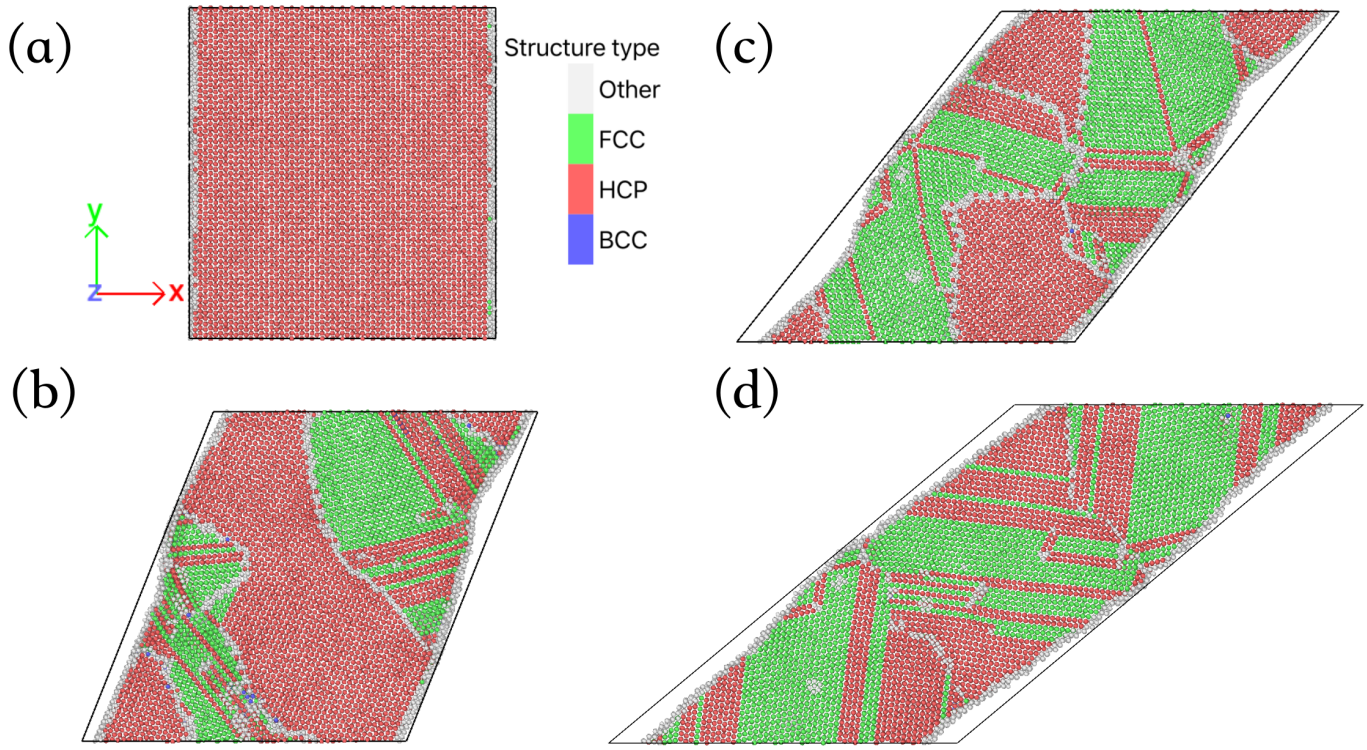

Fig. 5 Structural evolution under shear loading at shear strain of (a) 0, (b) 0.4, (c) 0.8 and (d) 1.2. The red color represents atoms in HCP structure while green color represents atoms in FCC structure.

Notes and references

1 X. Zhou, R. Johnson and H. Wadley, Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers, *Physical Review B*, 2004, **69**, 144113.

2 S. Zhao, Y. Xiong, S. Ma, J. Zhang, B. Xu and J.-J. Kai, Defect accumulation and evolution in refractory multi-principal element alloys, *Acta Materialia*, 2021, **219**, 117233.