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Supplementary information

Probing microstructure and deformation mechanism of FeCoCrNiAl0.5 high entropy alloy

during nanoscratch: A combined atomistic and physical model study Yong Zhang^{a,b*}, Wenfei Yang^b, Jing Peng^{c*}, Andong Wang^b, Weijie Fan^b, Jia Li^c

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Figure S1 The surface morphology of FeCoCrNiAl_{0.5} HEA with different scratching distances: (a) 10 nm, (b) 20 nm, (c) 30 nm, and (d) 36 nm. Atoms are colored according to the atomic height.



Figure S2 The displacement distribution in the pure Ni for the scratching distance: (a) 10 nm, (b) 20 nm, (c) 30 nm, and (d) 36 nm.



Figure S3 The strain distribution in the pure Ni for the scratching distance: (a) 10 nm, (b) 20 nm, (c) 30 nm, and (d) 36 nm.



Figure S4 The evolution of instantaneous microstructure in the pure Ni for the scratching distance: (a) 10 nm, (b) 20 nm, (c) 30 nm, and (d) 36 nm.



Figure S5 The dislocation evolution with the scratching distance: (a) 10 nm, (b) 20 nm, (c) 30 nm, and (d) 36 nm. (green line), <100> (pink line), <110> (blue line), and other (-

red line) dislocations in the upper row. The — blue lines stand for the edge dislocations, the — red lines stand for screw dislocations, and other color lines stand for the mixed dislocations in the lower row.



Figure S6 The distribution of (a) displacement, and (b) shear strain for different scratching depths: 0.5 nm, 1.5 nm, and 2.0 nm in the pure Ni.



Figure S7 The distribution of stress for different scratching depths: 0.5 nm,1.0 nm, 1.5 nm, and 2.0 nm in the pure Ni.



Figure S8 The evolution of (a) surface morphology, (b) instantaneous microstructure and (c) dislocation for different scratching depths: 0.5 nm, 1.5 nm, and 2.0 nm in the pure Ni.