Electronic Supplementary Material (ESI) for Nanoscale Advances. This journal is © The Royal Society of Chemistry 2023



Fig.S0. Molecular dynamics simulation model of Fe14.6Ni (at %) alloy. Fe atoms were in red and Ni atoms were in blue.



Fig.S1. The XRD diffraction pattern of Fe14.6Ni(at%) alloy detected by experimental method and calculated by MD simulation



Fig.S2. The six stages of the stress-strain curve.



Fig.S3. The six stages of the temperature variation process. (a)The global view;(b) The local view.



Fig.S4. The six stages of the total kinetic energy variation process. (a)The global view;(b) The local view.



Strain

Fig.S5. The six stages of the phase content evolution processes.