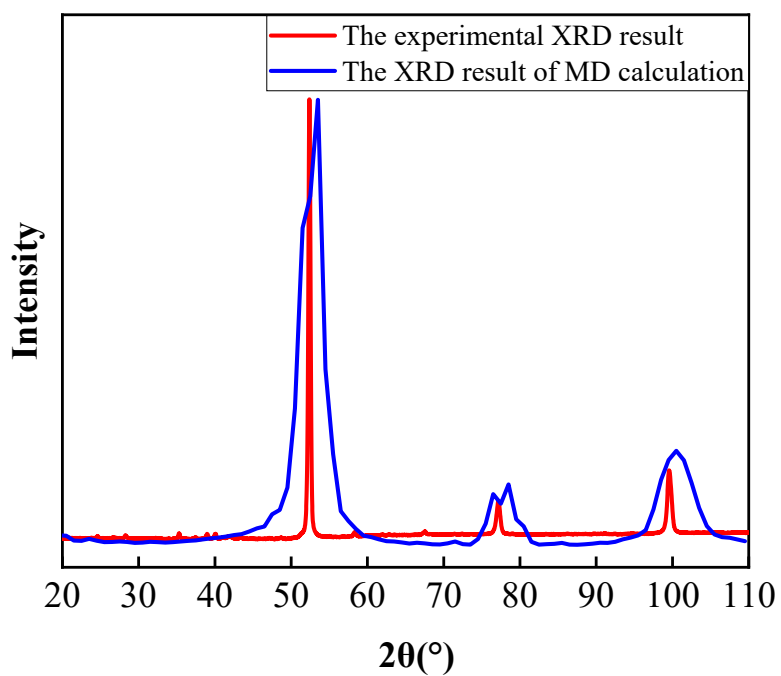


**Fig.S0.** Molecular dynamics simulation model of Fe<sub>14.6</sub>Ni (at %) alloy. Fe atoms were in red and Ni atoms were in blue.



**Fig.S1.** The XRD diffraction pattern of Fe<sub>14.6</sub>Ni(at%) alloy detected by experimental method and calculated by MD simulation

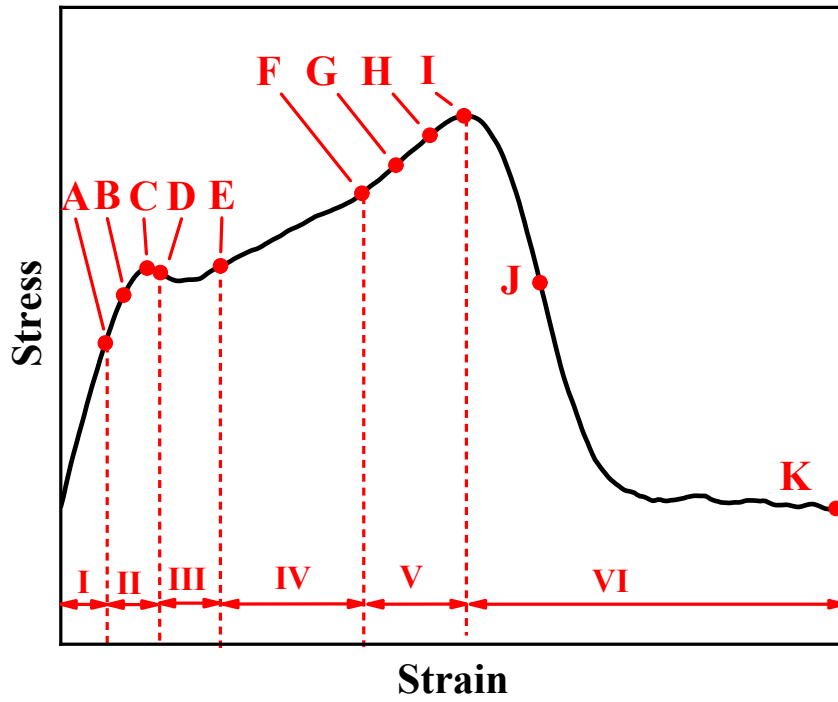


Fig.S2. The six stages of the stress-strain curve.

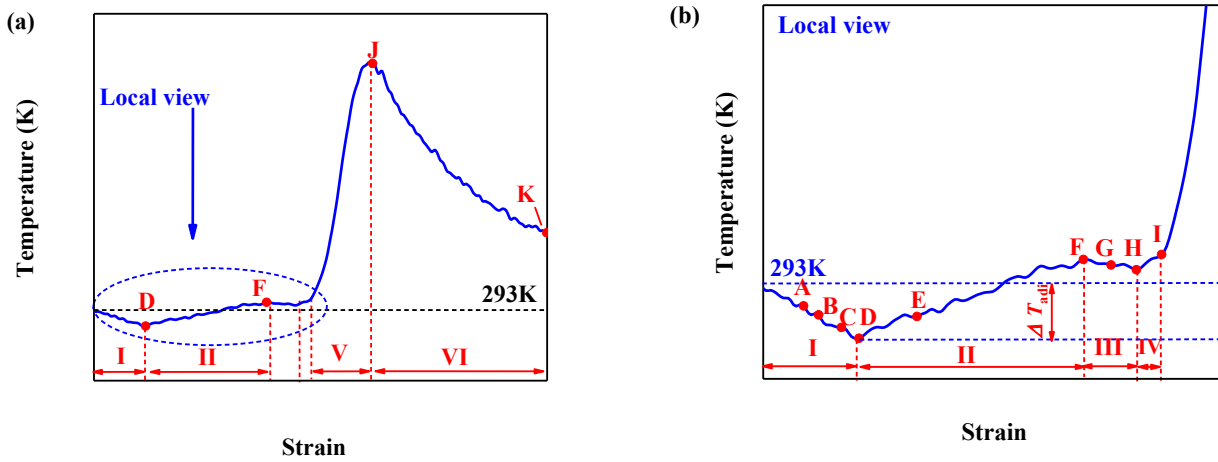


Fig.S3. The six stages of the temperature variation process. (a)The global view;(b) The local view.

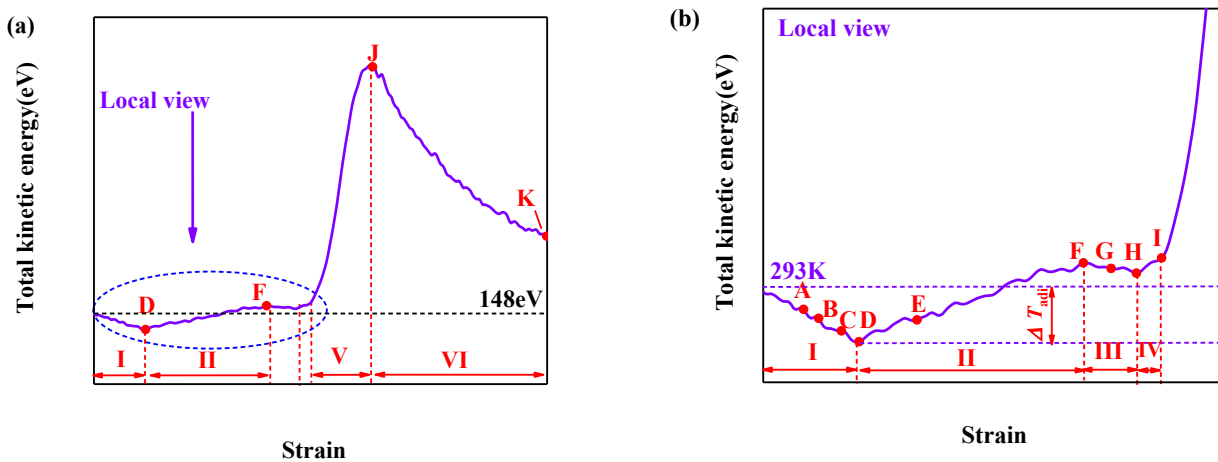


Fig.S4. The six stages of the total kinetic energy variation process. (a)The global view;(b) The local view.

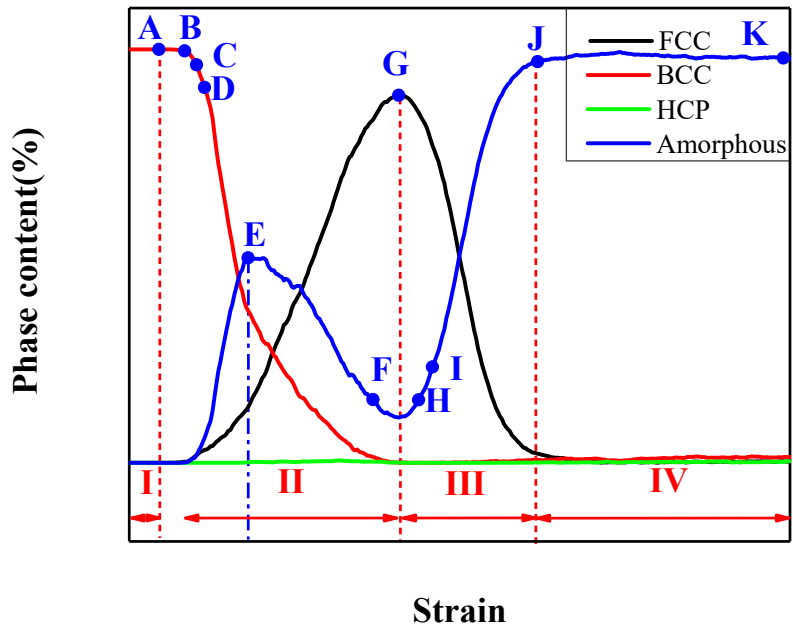


Fig.S5. The six stages of the phase content evolution processes.