Accepted Manuscript

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PII: S0749-6419(17)30007-4

DOI: 10.1016/j.ijplas.2017.04.016

Reference: INTPLA 2194

To appear in: *International Journal of Plasticity*

Received Date: 3 January 2017

Revised Date: 27 March 2017

Accepted Date: 19 April 2017

Please cite this article as: Wang, K., Chen, J., Zhu, W., Hu, W., Xiang, M., Phase Transition of Iron-based Single Crystals under Ramp Compressions with Extreme Strain Rates, *International Journal of Plasticity* (2017), doi: 10.1016/j.ijplas.2017.04.016.

Phase Transition of Iron-based Single Crystals under Ramp Compressions with Extreme Strain Rates

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Abstract

Recent widespread interests on strain rate effects of phase transition under dynamic loadings bring out present studies. α→ε phase transition of iron, as a prototype of martensite phase transition under dynamic loadings, exhibits huge diverges in its transition pressure (TP) among experiments with different pressure medium and loading rates, even in the same initial samples. Great achievements are made in understanding strain or stress dependence of the TP under dynamic loadings. However, present understandings on the strain rate dependence of the TP are far from clear, even a virgin for extreme high strain rates. In this work, large scale nonequilibrium molecular dynamics simulations are conducted to study the effects of strain rates on the phase transition of iron-based single crystals. Our results show that the phase transition is preceded by lattice instabilities under ramp compressions, but present theory, represented by modified Born criteria, cannot correctly predict observed onsets of the instability. Through considering both strain and strain gradient disturbances, new instability criteria are proposed, which could be generally applied for studying instabilities under either static or dynamic loadings. For the ramp with a strain rate smaller than about 10^{10} s^{-1}, the observed onset of instabilities is indeed equal to the one predicted by the new instability criteria under small gradient disturbances. The observed onsets deviates from the predicted one at lager strain rates because of finite strain gradient effect —— nonzero higher order stresses and work conjugates of the strain gradient. Interestingly, the strain rate ($\dot{\varepsilon}$) dependence of the TP also exhibits an obvious change at the same strain rate, i.e., 10^{10} s^{-1}. When $\dot{\varepsilon} \leq 10^{10}$ s^{-1}, a certain power law is obeyed, but it is not applicable at larger strain rates. This strain rate effect on the TP are well interpreted with nucleation time and the finite strain gradient effect. According to these basic understandings, the roles of strain rates on nucleation and growth of the phase transition are studied. Besides, initial shock formation time at extreme strain rates is analyzed, which also exhibits a deviation from a scaling law.

Key Words: Phase transition; Strain rate; Strain gradient; Lattice instability; Molecular dynamics; Ramp compressions; Metal.

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