

[PO-C1]Poster Session 1

Symposium C

Mon. Oct 29, 2018 5:45 PM - 8:00 PM Poster Hall

[P1-09]Structural and magnetic properties of long-period stacking ordered (LPSO) structure of iron; A first-principles study

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Fe-Mn-Si based alloys is known to exhibit a shape-memory effect associated with deformation-induced martensitic transformation from face-centered cubic (fcc) γ -austenite to hexagonal closed packed (hcp) ϵ -martensitic phase. The Fe-Mn-Si-based alloys with modified chemical compositions appeared to have outstanding properties of low-cycle fatigue lives, and a Fe-15Mn-10Cr-8Ni-4Si (mass%) alloy developed is practically used in a seismic damping component of architectural constructions. Recently, under cyclic push-pull loading of Fe-Mn-Si-based alloys, a new phase different from ϵ -phase was found by transmission electron microscopy. The new phase shows electron diffraction spots at the $1/3$ position of the $\{10\bar{1}1\}$ spots of the ϵ -phase, which suggests the existence of a long-period stacking ordered (LPSO) structure. In 1960s, a similar phase was reported after several times of thermal cycles of γ - ϵ phase phase transitions in Fe-Mn-C alloys. However, actual stacking sequence of the LPSO phase and relative stability with γ and ϵ -phases still remain unclear. To understand these issues, we proposed several structural models of LPSO structure of pure Fe, such as $4H$, $6H_1$ and $6H_2$, and discuss structural and magnetic stabilities among the candidate of LPSO structures with first-principles calculation methods. [1] L. I. Lysak, and B. I. Nikolin, *Fiz Met. Mettaloved* **20**, 547 (1965), *ibid.* **23**, 93 (1967).