Dominates roles of valence electron concentration and ferromagnetism on precipitation in NiFeGa magnetic shape memory alloys

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Abstract

In Heusler-type functional alloys, incorporating ductile precipitates stands as an effective method to reduce brittleness, a major limitation hampering their practical applications. Uncovering the physical origin behind precipitation and the key factors deciding to tailor precipitation behaviors hold immense significance. To this end, by combining first-principles calculations and experimental examinations, the precipitation in Ni2FeGa was systematically studied. The primary discoveries are as follows: The matrix with L21 structure in Ni2FeGa exhibits poor elastic and dynamic stabilities, potentially linked to the occurrence of precipitation. Theoretical and experimental assessments identify the precipitates as having an L12 structure instead of the commonly reported FCC structure. This structural preference is elucidated by the electron density of states and chemical bond considerations. Slight element partitioning, enriching Fe and depleting Ga in precipitates, accelerates the driving force for precipitation. Notably, the stability of the precipitate against the matrix is influenced by valence electron concentration (e/a) and magnetism, displaying sensitivity coefficients of -175.1 and 67.4 meV, respectively. Increased e/a stabilizes the precipitate, while enhanced magnetism favors the matrix. In contrast, the impact of lattice volume on precipitation is minimal concerning both sensitivity and adjustment range. A strategy for modulating precipitation by adjusting e/a and magnetism has been proposed and confirmed. This work is expected to lay a solid foundation for precipitation engineering of Heusler alloys and thus to facilitate the design of advanced precipitate-enhanced ferromagnetic Heusler materials.

Keywords: Magnetic shape memory alloy, Precipitation, Valence electron concentration, Ferromagnetism, First, principles calculation

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