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Influence of atomic order on the enthalpy of formation and bulk modulus of the sigma phase

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Abstract

We have calculated the enthalpy of formation and bulk modulus for 19 typical binary sigma compounds with different atomic order (i.e. atomic constituent distribution or site occupancy preference on inequivalent sites of a crystal structure) based on the experimental site occupancy as well as completely ordered and hypothetically disordered states by using the EMTO-CPA (Exact Muffin-Tin Orbitals - Coherent Potential Approximation) method. The calculation results show that at 0 K the sigma phase in ordered state bears a lower enthalpy of formation and a larger bulk modulus than the ones in less ordered state.

Key words: sigma phase, atomic order, enthalpy of formation, bulk modulus, EMTO-CPA

1. Introduction

The topologically close-packed (TCP) phases are one of the largest groups of intermetallic compounds, which are composed of metallic atoms with different atomic size. These atoms adapt each other forming a very complex crystal structure with high space utilization and high coordination number (CN). The characteristic of the structure is that it is stacked by coordination polyhedron of CN 12, 14, 15 and 16 [1]. TCP phase is common precipitation in Fe-, Ni-, Co-based superalloys and austenitic and duplex stainless steels [2–5]. The common members of TCP phases are sigma, chi, mu, laves, A15, R, P, delta and M phases [1,2]. A small amount of TCP precipitations can cause the effect of precipitation hardening and grain boundary strengthening [3,6]. However, in most cases, TCP phase is a detrimental phase in alloys. It is hard and brittle, which make alloys crack under the service conditions in tensile stress. Moreover, the TCP precipitation will lead to poor alloying elements in matrix, and thus decreases the mechanical properties and corrosion resistance of materials [2,3]. Therefore, accurate prediction and reasonable control of the precipitation of TCP phase is obviously the key to alloy design of iron-based, nickel-based, cobalt-based superalloys and stainless steels.

The sigma phase is a typical example of TCP phases, which is with large homogeneity range and designated as tetragonal