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Diffusion in Ni-Based Single Crystal Superalloys with Density Functional Theory and Kinetic Monte Carlo Method

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Abstract. In the paper, we focus on atom diffusion behavior in Ni-based superalloys, which have important applications in the aero-industry. Specifically, the expressions of the key physical parameter – transition rate (jump rate) in the diffusion can be given from the diffusion theory in solids and the kinetic Monte Carlo (KMC) method, respectively. The transition rate controls the diffusion process and is directly related to the energy of vacancy formation and the energy of migration of atom from density functional theory (DFT). Moreover, from the KMC calculations, the diffusion coefficients for Ni and Al atoms in the γ phase (Ni matrix) and the γ' phase (intermetallic compound Ni_3Al) of the superalloy have been obtained. We propose a strategy of time stepping to deal with the multi-time scale issues. In addition, the influence of temperature and Al concentration on diffusion in dilute alloys is also reported.

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Key words: Diffusion behavior, transition rate, density functional theory, kinetic Monte Carlo method, superalloy.

1 Introduction

Diffusion in solids, a fundamental phenomenon in material science, involves the correlation behavior of atomic motion and multi-length and time scales. In this paper, we focus

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on the factors influencing the properties of Ni-based superalloys doped with heavy element Re, which have important applications in the aero-industry [1–11]. Motivated by scientific interest in superalloys, our work concerns the density functional theory as well as the diffusion behavior in solids [12–18].

Diffusion in superalloys is closely related to the evolution of the structural system, which involves its phase stability and homogenization, as well as the precipitation and dissociation of phases. In particular, the diffusion of atoms directly influences the high temperature creep behavior and thermal oxidation properties; we need to understand its mechanism and to control the process. In metals and alloys, the diffusion mechanism concerns mainly point defects induced by thermal fluctuations. Vacancy mechanism has been considered as the dominant mechanism in metals [19]. In this work, we confine our study to the atomic jump process of diffusion in matrix Ni and its dilute substitutional binary alloy [19], and study the diffusion process in $L1_2$ intermetallic Ni_3Al via the sublattice vacancy mechanism [19–21] for Ni atoms and Al atoms.

Kinetic Monte Carlo (KMC) methods [22, 23] are used in computations in many areas that study the dynamic behavior of systems with interacting particles. By describing the configuration transition process instead of calculating atom trajectories, the KMC method can provide a multi-time and multi-length scale description for the diffusion behavior of materials. For each step in the algorithm, an atomic transition process is chosen at random from a list of possible processes; the probability for each process is weighted by its transition rate (jump rate). A previous theoretical study [24] has shown that, under some general conditions, the KMC method simulates both the static and dynamic properties of model systems consistently and correctly. In contrast, molecular dynamics simulations describing the trajectories of individual atoms or molecules on potential energy are not computationally capable of probing large systems of interacting particles over long times. Thus, in a dynamics capacity, the KMC methods are an efficient means for studying diffusion that bridges density functional theory (DFT) and dynamic approaches. The predictive power of the KMC methods has been demonstrated for a wide range of experimental phenomena, such as vacancy diffusion [25], phase transition [26], domain growth [27], and adatom diffusion on surface [28–30]. In addition, these methods are of crucial importance to the study of electron transport in organic materials [31, 32].

In this paper, the theoretical basis is on the harmonic transition state theory (HTST) [22, 23, 32, 33] and to calculate KMC transition rate with DFT. The HTST transition rate trends to a very exact rate in most solid materials for solid state diffusive processes [34, 35].

2 Construction of calculation model with relevant experiments

Motivated by scientific interest and the importance of properties of Re-doped Ni-based superalloys (considering the solubility of Re from the phase diagram of Ni-Al-Re system and the lower content of Re, the more interesting for superalloys), as indicated by exper-