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Crystal-melt kinetic coefficients of Ni₃AlR. Ramakrishnan¹, R. Sankarasubramanian^{*}

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ABSTRACT

Crystal-melt interface growth kinetics of the intermetallic system, Ni₃Al, is investigated using molecular dynamics simulation. Kinetic coefficient, one of the important parameters that controls solidification growth morphology, is calculated using free solidification method employing two different interatomic potentials. Compared to pure metals, the kinetic coefficients of the ordered systems are smaller by at least an order of magnitude. For the first time, we show here that the growth kinetics of ordered Ni₃Al is very sluggish compared to that of the disordered system. The difference is attributed to the diffusion limited growth in the ordered systems vis-à-vis the interface limited growth in their counterpart. Theoretical models by Broughton-Gilmer-Jackson and Wilson-Frenkel are employed to corroborate the identified growth mechanisms. The extent of disorder trapped increases with increasing interface velocity.

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1. Introduction

Kinetic coefficient, μ , is the proportionality constant between the solid-liquid interface velocity, v , and undercooling, ΔT , and is known to affect the morphology of dendrites to a large extent [1]. Till date, very few direct experimental measurements of μ have been reported [2,3]. Rodway and Hunt [3] developed a method based on Seebeck effect to measure interface velocity-undercooling relation and obtained a value of 28 cm/s-K for Pb. Also, there are solidification studies on dendrite growth velocities of levitated droplets, at specific undercoolings for various metallic systems [4–6].

The interface velocity is dependent on the crystallographic plane of the solid interfacing with the liquid. As a result, kinetic coefficient can have anisotropic dependence which in turn would result in the preferential growth of certain crystallographic planes over the others leading to highly faceted solidified microstructures. However, it is rather very difficult to determine the anisotropy in kinetic coefficients through experimental means.

With the availability of accurate interatomic potentials and computational resources, molecular dynamics (MD) simulation has been widely used in calculating the kinetic coefficients. A review by

Hoyt et al. [7] explains different methods by which the kinetic coefficient can be calculated using MD. Most of the studies on pure elements such as Ni [8–10], Cu [9,10], Au [11,12], etc suggest existence of strong anisotropy in kinetic coefficients with (1 0 0) plane having the highest growth rates. Monk et al. [8] have investigated the effect of simulation methodologies such as thermostats on the estimation of kinetic coefficients. Mendelev et al. [9] have compared the kinetic coefficients in fcc metals (Ni, Al and Cu) calculated using various interatomic potentials. Ashkenazy and Averbach [13] have reported that in bcc and fcc metals, a cross over temperature T_c , separates the thermally activated (diffusion controlled) and athermal growth regimes.

Kinetic coefficients calculated for B2-NiAl intermetallic [14–17] shows that they are at least an order of magnitude lower than those of pure elements. Zheng et al. [16] have studied B2-NiAl compound during solidification to investigate disorder trapping and have reported significantly less anisotropy in the measured interface velocities. Tang and Harrowell [17] have reported that glass forming alloy, CuZr has significantly lower growth rate and interface width than NiAl, a poor glass former alloy. Ovrutsky et al. [15] have studied the mechanism of nuclei formation in B2-NiAl using MD simulation and reported interface velocities at different undercoolings. While the above mentioned studies have focused on ordered systems, the dependence of growth kinetics on undercooling and solute content in disordered systems, viz., Ni-Si [18] and Ni-Zr [19] has also been investigated. However, there is no report on how the kinetic coefficient varies between the solidification of ordered

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and disordered intermetallics.

B2-NiAl and Ni₃Al (L1₂) are intermetallic phases present in technologically important materials for aeroengine components made from nickel base alloys. Knowledge of the solidification kinetics of these compounds will aid in simulating the morphological evolution of microstructures using techniques such as phase field method. To the best of the knowledge of the authors, there is no published report on the kinetic coefficient of Ni₃Al and how significantly it could vary between the solidification of ordered and disordered structures. In the present study, we report our calculations on the kinetic coefficients of Ni₃Al intermetallic system using two different interatomic potentials. The use of two different potentials has facilitated us to study the difference in the kinetics of solidification of ordered and disordered Ni₃Al. The next section describes the computational methodology used for calculating the kinetic coefficients. Results of our calculations are discussed in detail in section 3.

2. Computational methodology

MD simulations are carried out using an open source software package “LAMMPS” (Large scale Atomic/Molecular Massively Parallel Simulator) developed at Sandia National Laboratory [20]. Free solidification method [7] is employed to calculate crystal-melt interface kinetic coefficient. Throughout the work, periodic boundary conditions are used to simulate bulk system behavior and the details of the investigated systems are given in Table 1.

Initially, a rough estimate of the melting temperature is obtained using step-wise progressive heating of a bulk crystal. The temperature at which there is an abrupt change in the energy (because of latent heat release) or the volume of the system is an indication of melting and this temperature is generally expected to be higher than the exact melting temperature. This is because, in the absence of any nuclei, the solid needs to be superheated before melting. For the exact determination of the melting temperature (T_m), coexistence method [21] is used. Here, a system geometry is chosen in such a way that the length is at least five times than that of the other two dimensions. Half of the system in the length direction is equilibrated at a temperature below, and the other half above, the estimated melting temperature. NPT ensemble (constant number of atoms, pressure and temperature) is used in this procedure and the entire cell is maintained at zero external pressure. Equilibration is achieved by carrying out MD simulations for 300 ps. A timestep of 1 fs is considered throughout this work. The resulting solid-liquid system is further relaxed under canonical ensemble (NVT) for about 300 ps with temperatures of the regions being the same as used in the NPT ensemble. This procedure relaxes the system pressure at a constant volume. This is followed by an equilibration step for about 3–5 ns in microcanonical (NVE) ensemble. This equilibration will result in a configuration containing either a complete solid or a complete liquid or both solid and liquid phases, depending on the pressure-temperature combinations. Essentially, from this NVE run, combinations of pressures and temperatures corresponding to coexisting solid and liquid

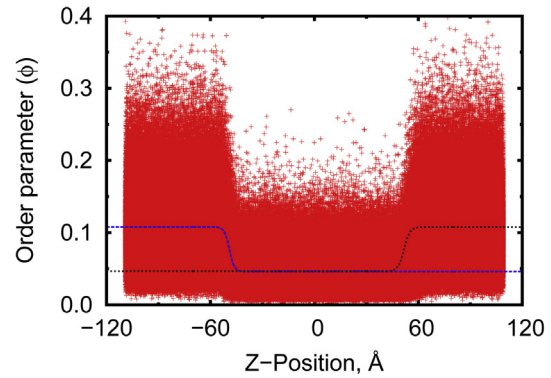


Fig. 1. Variation of structural order parameter of Ni₃Al (Potential 1) with respect to the coordinate perpendicular to the solid-liquid interface.

phases (P-T phase diagram) are obtained. Pressures and temperatures are averaged over simulation runs spanning over 1 ns for conditions under which both solid and liquid phases are stable. From this coexistence method [21], zero pressure melting temperature is obtained.

The system configurations which are at equilibrium melting conditions are further considered as the initial configurations for the free solidification simulations. The entire solid-liquid system is equilibrated using NPT ensemble with zero external pressure and at various temperatures below and above T_m . To account for statistical variations, at least six different randomly selected initial solid-liquid configurations are considered in this study. Solidification (melting) is characterized by a decrease (increase) in the system energy as a function of time.

The interface velocity is calculated by tracking the position of the interface as a function of time. In order to locate the interface, a structural order parameter, $\phi = \frac{1}{12} \sum_i |r_i - r_{fcc}|^2$ that distinguishes the solid and the liquid regions is used. Here, for a given atom, r_i denotes the distances of the first 12 neighbors in the simulated structure and r_{fcc} refers to the first nearest neighbor distance for the ideal fcc crystal. This definition [22] ensures that $\phi \approx 0$ for the fcc solid and nonzero for the liquid regions. The position of the interface at any snapshot is identified by fitting a function $c_1 + c_2 \tanh((z - c_3)/d)$ (see for example Fig. 1), where z is the coordinate of the atoms along the longer axis of the system (perpendicular to the solid-liquid interface) and the fitting parameter, c_3 denotes the interface position [16].

In this study, the embedded atom method potential for Ni-Al system from two different publications are used; (i) by Mishin et al. [23] referred to as Potential 1 and (ii) by Pun and Mishin [24] referred to as Potential 2, in the rest of this paper. Low index planes, viz., (0 0 1), (1 1 0) and (1 1 1) of the solid interfacing with the liquid are considered to calculate the kinetic coefficients of Ni₃Al. For the sake of completeness, we also report the results for Ni, Al and B2-NiAl. The starting configurations of the solid in the case of

Table 1
System geometries used in the simulations.

Crystal plane interfacing with liquid	X	Y	Z	Size range for different systems, Å	Number of atoms	
					in Ni, Al and L1 ₂ -Ni ₃ Al systems	in B2-NiAl system
(0 0 1)	[1 0 0]	[0 1 0]	[0 0 1]	34.3 × 34.3 × 171.5–42.3 × 42.3 × 211.6	34560	17280
(1 1 0)	[0 0 1]	[1 $\bar{1}$ 0]	[1 1 0]	34.3 × 32.3 × 161.7–42.3 × 39.9 × 199.5	30720	15360
(1 1 1)	[1 $\bar{1}$ 0]	[1 1 $\bar{2}$]	[1 1 1]	40.4 × 42.0 × 198.1–49.9 × 51.8 × 244.3	57600	28800

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