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Comparison of coarsening behaviour in non-conserved and volume-conserved isotropic two-phase grain structures

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ABSTRACT

Microstructure evolution in non-conserved and volume-conserved isotropic two-phase grain structures, with equal interfacial energy for all interfaces and equal volume fractions of the two-phases, is compared based on large-scale phase-field simulations. Two important observations are as follows: (1) the growth mechanism has a larger effect on the grain size distributions of the two alloys than on their grain topology distributions; (2) the growth rate and normalized grain size relation of the grains per topological class are much more scattered for the conserved system than the non-conserved system.

Two-phase polycrystalline materials can offer better material properties, like high strength, toughness and corrosion resistance over single-phase polycrystalline materials. A two-phase microstructure, with α and β phases may contain α/α, β/β and α/β interfaces. Cahn [1] analyzed the stability of various microstructural features for two-dimensional (2D) non-conserved two-phase (NCTP) systems. It was found that the energetic ratios $\sigma_\alpha/\sigma_{\alpha|\beta}$ and $\sigma_\beta/\sigma_{\alpha|\beta}$, with σ_α, σ_β and $\sigma_{\alpha|\beta}$ the energies of the α/α, β/β and α/β interfaces respectively, control the stability, spatial distribution and grain shapes of the 2 phases in a two-phase system. This was later confirmed by Holm et al. [2] with Monte Carlo-Potts simulations for the 2D NCTP systems. Furthermore, Cahn [1] extended the von Neumann-Mullins law [3,4], which describes an exact relation between the rate of change of grain area (dA/dt) of an individual grain and its number of sides (F) in the 2D isotropic single-phase systems, to the 2D isotropic NCTP systems. Cahn [1] also suggested that a further extension of the von Neumann-Mullins law to 2D volume-conserved two-phase (VCTP) systems would be a formidable mathematical problem. Fan and Chen [5,6] performed simulations for 2D VCTP and speculated that the modified von Neumann-Mullins law proposed by Cahn [1] may apply to 2D two-phase systems in general [6]. Holm et al. [2] also suggested that the microstructures of the NCTP and VCTP systems in 2D and 3D with equal volume fraction ($V_\alpha = V_\beta = 0.5$) will be structurally equivalent, as the triple junction stability criteria in 2D and triple line stability criteria in 3D for the NCTP and VCTP alloys are the same. However, in a previous study [7], it was observed that various microstructural features in the NCTP and VCTP systems are influenced by the different growth controlling mechanisms and growth kinetics. The goals of the present work are (1) to compare microstructure evolution; (2) to test the applicability of the von Neumann-Mullins law in 2D; and (3) to compare volumetric growth rates in 3D for isotropic NCTP and VCTP systems with $V_\alpha = V_\beta = 0.5$. Furthermore, $\sigma_\alpha = \sigma_\beta = \sigma_{\alpha|\beta}$, was chosen so that the growth kinetics in the NCTP alloy and single-phase system is identical.

A two-phase phase-field model was employed to carry out large-scale simulations for the NCTP and VCTP systems [7]. Further details on simulations can be found in [7], where the effect of the volume fractions on volume-conserved isotropic two-phase coarsening was studied. The 50/50 alloy in [7] is renamed as VCTP alloy in the present study. Some microstructural features of NCTP and VCTP systems were discussed in brief and the summary of this discussion in [7] are as follows: (1) a growth exponent $n \sim 2$ for the NCTP alloy and $n \sim 3$ for the VCTP alloy was found in the 2D and 3D simulations; (2) All four types of triple junctions (TJs) namely $\alpha\alpha\alpha$, $\alpha\alpha\beta$, $\alpha\beta\beta$, and $\beta\beta\beta$ TJs are present in equal volume fraction in the NCTP alloy, whereas there are less $\alpha\alpha\alpha$ and $\beta\beta\beta$ TJs than $\alpha\alpha\beta$ and $\alpha\beta\beta$ TJs in the VCTP alloy in 2D simulations; and (3) In the 2D VCTP alloy, most of the grains with 3 and 4 sides had a grain size comparable to the mean grain size $\langle R \rangle$, whereas, in the 2D NCTP alloy, most of the grains with 3 and 4 sides had a grain size smaller than the $\langle R \rangle$. The grain size

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distributions (GSDs) and grain topology distributions (GTDs) of the total grain structure ($\alpha + \beta$ phase grains) for the NCTP and VCTP alloys were only discussed very briefly and not compared in [7].

Thus, in the present study, further analysis related to the GSDs and GTDs was carried out first. The GSDs obtained for the NCTP alloys are found to be significantly wider than those obtained for the VCTP alloys in both the 2D and 3D simulations as shown in Fig. 1a and b. For the 2D simulations, the shape of the GSD for the NCTP alloy is close to that obtained previously from grain growth simulations for a single-phase system [8–10]. Similarly for the 3D simulations, the GSD for the NCTP alloy matches that obtained from previous single-phase grain growth simulations [8,11,12]. The GSD obtained for the VCTP alloy in 3D simulations matches the GSD obtained for solid particle coarsening in a liquid matrix with a volume fraction of the solid particles of 0.78 [13]. The Weibull distribution (with $\beta = 3.035$) gave a good fit to the GSD of the VCTP alloy, whereas the Rios distribution (with $\nu = 3.2$) gave a good fit to that of the NCTP alloy [14]. The GTDs are shown in Fig. 1c and d. For 2D simulations, the GTD is peaked around $F = 6$ for the VCTP alloy, whereas it is peaked between $F = 5$ and $F = 6$ for the NCTP alloy, which is in agreement with previous studies [8,15] for single-phase grain structures in 2D. In the 3D simulations, the GTDs obtained for the NCTP and VCTP alloys are similar except towards the tail (at high F) where the VCTP alloy has fewer grains with $F \geq 30$ than the NCTP alloy. The GTDs obtained from the 3D simulations match those obtained in previous experimental [16,17] and simulation [8,11,12] studies. Thus, the difference in growth mechanism and growth kinetics in the NCTP and VCTP alloys has a stronger influence on the GSDs than on the GTDs.

The evolution of individual grains in the isotropic 2D single-phase system is exactly described by the von Neumann-Mullins law [3,4], which is given as

$$\frac{dA}{dt} = -m\sigma\frac{\pi}{3}(6 - F), \tag{1}$$

where A is the area of a given grain, t is time, m is grain boundary mobility, σ is grain boundary energy and F is the number of sides of the considered grain. According to Eq. (1), the rate of change of the area of an individual grain depends only on its number of sides F. Thus, all grains with $F > 6$ will grow, while all grains with $F < 6$ will shrink and all grains with $F = 6$ will not change size and remain stable. Eq. (1) was extended by Cahn [1] for two-dimensional non-conserved isotropic two-phase systems. It was also shown [1] that the modified von Neumann-Mullins law reduced to Eq. (1) when $\sigma_\alpha = \sigma_\beta = \sigma_{\alpha/\beta}$ (which is equivalent to the NCTP alloy in the present study). In Fig. 2a and b, the rates of area change dA/dt of all the grains, as obtained from the 2D simulations, are plotted against their normalized grain sizes ($R/\langle R\rangle$) for the NCTP and VCTP alloys. For the NCTP alloy, the data points obtained for grains of a same topological class are located along a horizontal line (see Fig. 2a), indicating that the dA/dt is similar for all grains from the same topological class independent of the grain size. However, for the VCTP alloy, there is a considerable scatter on the data points obtained for grains of a same topological class (see Fig. 2b). This contrast between 2D NCTP and VCTP alloys is again seen in Fig. 2e and f where the average and standard deviation of the dA/dt data for a given F is plotted. It is clear that the standard deviation within a given topological class is much larger in the VCTP alloy than the NCTP alloy. These results show that, for the 2D VCTP alloy, the von Neumann-Mullins law (1) is only valid for the average of dA/dt as a function of F and not for the growth rate of the individual grains. Our findings for the 2D NCTP system are consistent with previous observations from 2D single-phase systems [10]. It is important to note that the small variation among the growth rates of the individual grains of a given topological class for the NCTP alloy seen in the simulations is due to numerical inaccuracies. As pointed out in [10], whenever a shrinking grain has a size comparable to the diffuse interface width in a phase-field model, its kinetics are affected. This may have some influence on the kinetics of the neighbouring grains, explaining the slightly larger variations in growth rates as compared to [18]. The variations for a given topological class for 2D NCTP are similar to those in the Kim et al. [10] study.

In Fig. 3, we show the evolution of the area and number of sides of 2 individual grains as a function of time for the VCTP alloy. Grain A

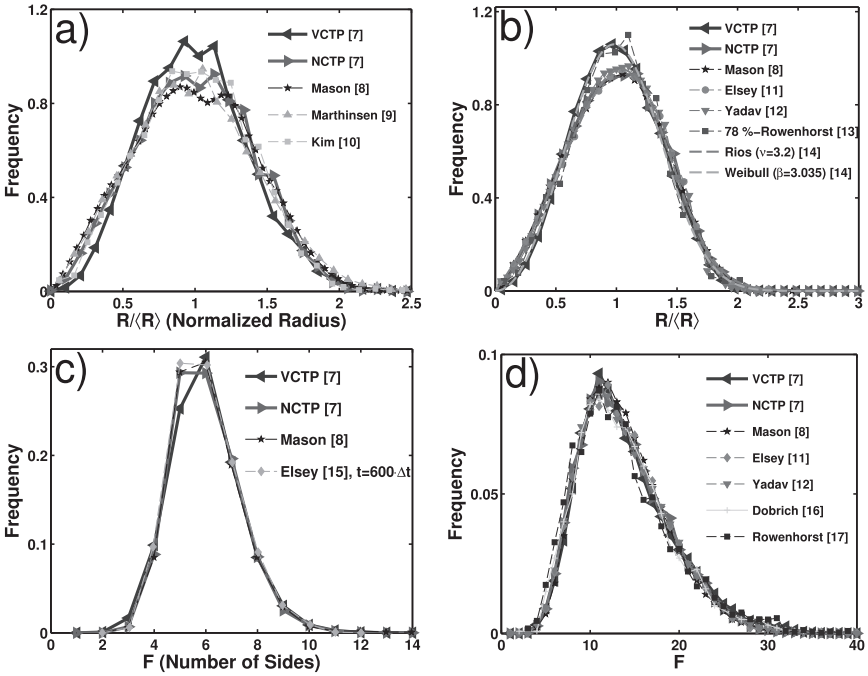

Fig. 1. Grain size and grain topology distributions for the VCTP and NCTP alloys in 2D and 3D. a and b show the GSDs in 2D and 3D respectively. Similarly, c and d show GTDs in 2D and 3D respectively. Results are compared with previous simulation [8-12,15], experimental [13,16,17] and analytical [14] results.