



Enhancement of thermal stability by microstructural refinement in nanocomposite materials

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The enhancement of thermal stability in nanocrystalline-amorphous (NC-*a*) materials was investigated by a modified Monte Carlo Potts method. The thermal stability, including the grain size stability and amorphous distribution stability, was found to be controlled by the amorphous fraction f and the energy ratio (J_{gb}/J_{int}) of the NC-NC grain boundary energy to the NC-*a* interfacial energy. The best thermal stability for temperatures up to 1550 K was observed with $f = 0.279$ and $J_{gb}/J_{int} = 12$, where finer grains are surrounded by thin and coherent NC-*a* boundaries.

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The thermodynamic stability of protective materials applied to the surfaces of metallic parts is significant in determining the usability, functionality and durability of machining tools, which are usually subjected to high temperatures. It is known that the excellent mechanical and structural properties of recently developed nanocomposite materials with microstructures comprising of nanocrystalline (NC) phase surrounded by amorphous (*a*) matrix is a simple consequence of the stability of their nanostructure and interface [1–3]. Therefore, the thermal stability of nanocomposites is crucial for the stability of nanostructures at elevated temperatures [4–7]. As an example, nanocomposite NC-TiN/*a*-BN films showed thermal stability up to ~250 K, whereas the pure TiN lost its stability at temperatures higher than ~750 K [8,9]. Two other promising nanocomposites, NC-TiN/*a*-Si₃N₄ and Ti-Al-Si-N, were observed to be stable up to ~1350 and ~1450 K, respectively [5,8,10]. These experimental results clearly suggest that the excellent thermal stability is strongly related to the phase configuration and microstructure, especially the grain size, amorphous fraction, grain boundaries and interfacial

boundaries. By carefully controlling the addition of elements (e.g. B in Ti-B-N and Si in Ti-Si-N), the microstructure of NC-NC grain boundaries and NC-*a* interfacial boundaries can be substantially modified, consequently enabling the engineered composites to operate at different temperatures with finer microstructure and suitable boundary mobility.

Previous experimental observations have shown the enhancement of thermal stability in nanocomposites vs. their counterpart single-phase materials [8,9]. However, the theoretical work on the phase configuration, inner grain growth, grain boundary and interfacial boundary interactions in nanocomposites under different thermal conditions is very limited. In addition, the thermal performance of nanocomposites under various temperatures and the influence of microstructure on the thermal stability remain unexplored. The present work investigates the thermal stability of a two-phase (NC-*a*) nanocomposite system by using Monte Carlo (MC) simulation based on a modified Q-state Potts model [11,12]. Our emphasis is to focus on the performance of nanocomposite materials with various additional elements and their amorphous fractions f under different temperatures by observing their microstructure after a given grain growth duration.

The continuum NC-*a* microstructure is mapped onto N^2 ($N = 200$) discrete triangular lattice sites. The

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number of lattice sites occupied by NC species is denoted as N_A and the fraction f of a phase is given by $(N^2 - N_A)/N^2$. Each lattice site is assigned two distinct spin states S and Q , where S represents the species ($S = 1$ for the NC species and $S = 0$ for the a species) and Q corresponds to the orientation state, with $Q = 1-50$ for the NC species and $Q = 0$ for the a species. The selected site will reorientate with a nearby site that has the same species but different orientations, or will exchange with neighbors that have different species. The total energy (E) of the system including the NC–NC grain boundary energy (E_{gb}) and the NC– a interfacial energy (E_{int}) can be calculated as Eq. (1) in Ref. [23].

J_{gb} and J_{int} are positive constants that are proportional to the isotropic E_{gb} and E_{int} , respectively. The site exchange or reorientation probability P depends on the Metropolis algorithm, i.e. $P = 1$ if $\Delta E \leq 0$, and $P = \exp(-\Delta E/k_B T)$ otherwise [11]. Here, ΔE is the system energy change associated with the event occurring, k_B is the Boltzmann constant and T is the temperature. Many studies have revealed the influence of simulation temperature on the grain size and grain size distribution [13–15]. In those works, T was not regarded as a real temperature. The feasibility of correlating the simulated grain growth with the real grain growth has been already realized and some investigations have successfully characterized the influence of the real temperatures on the evolution of microstructure using MC simulations [16–20]. In our work, we also treated T as real temperature on the Kelvin scale, and found that it is in good agreement with experimental work [5,8–10,21].

As mentioned in the calculation algorithm, the isotropic E_{gb} and E_{int} are scaled by J_{gb} and J_{int} , respectively. Therefore, the ratio of E_{gb} to E_{int} can be set as J_{gb}/J_{int} . We initially set the amorphous fraction $f = 0.063, 0.09, 0.115$ and 0.154 in the system with a fixed $J_{gb}/J_{int} = 4$ after a time duration of MCS (Monte Carlo step) = 5000. The initial grain sizes are the same for the systems with the same amorphous fraction.

Figure 1a shows the mean grain diameter (\bar{D}) of the NC– a system with various amorphous fractions f as a function of the simulation temperature T . It is evident that the temperature has a significant influence on the grain growth with low f values. For $f = 0.063$, the microstructure at lower temperatures possesses smaller grains and the grain growth is relatively evident at high temperatures. The inset shows the grain size evolutions for $f = 0.063$ at $T = 450$ and 950 K, respectively. However, the temperature-induced grain size increment gradually abates with increasing f . For $f = 0.154$, \bar{D} increases slightly when the temperature is increased from 300 to 1100 K. It is interesting to note that the addition of amorphous phase can enhance the grain size stability even at high temperatures. Figure 1b, c and d, e show details of the microstructural evolution in the NC– a systems with $f = 0.063$ and 0.154 , respectively, at $T = 1100$ K. There is a slight increase in grain sizes with $f = 0.154$ at high temperatures (Fig. 1d, e), while a more pronounced grain growth can be found at high temperatures with $f = 0.063$ (Fig. 1b, c). At an initial stage of the grain growth for $f = 0.063$, the smaller grains are almost surrounded by the NC–NC grain boundaries, while the larger grains are surrounded by mixed parts

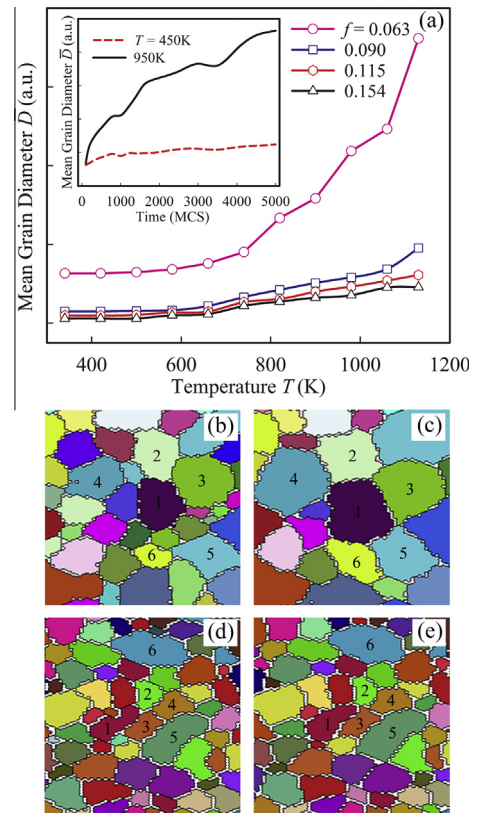


Figure 1. (a) Simulated mean grain diameter \bar{D} as a function of temperature T with various amorphous fractions f . The insets are the grain size evolutions of the system with $f = 0.063$ at $T = 450$ and 950 K, respectively. Microstructural evolutions with $f = 0.063$ (b, c) and $f = 0.154$ (d, e) at $T = 1100$ K.

of NC–NC grain boundaries and NC– a interfacial boundaries, respectively. During growth, smaller grains disappear, accompanied by the rapid growth of larger grains by directly swallowing smaller ones, as shown in the random grains numbered 1–6 in Figure 1b, c. For $f = 0.154$ as shown in Figure 1d, e, the increased area of NC– a interfacial boundaries becomes more coherent, constraining the grain growth substantially. It can be seen that grains 1–5 of Figure 1e are clearly separated by the coherent and thin amorphous phase. There is strong evidence that the grain growth behavior and the microstructure have a close relationship with the performance of nanocomposite materials at various temperatures. The results obtained above are in accordance with the experimental data of NC–TiN/ a -Si₃N₄ and NC–TiN/ a -BN, which demonstrate that the thermal stability is largely dependent on the silicon and boron contents, respectively [5,8–10,21].

Although increasing the amorphous fraction f can increase the area of the NC– a interfacial boundaries and reduce the grain size substantially, it does not necessarily mean that a greater value of f is always preferred. Either lack of or excess of the amorphous phase may lead to a decrease in the thermal stability. Evidence was obtained by studying the maximum stable temperature with different values of f for a typical value of $J_{gb}/J_{int} = 4$, shown in Figure 2. The maximum stable temperature refers to the temperature at which the nanocomposite system can maintain stable with a constant grain size rather than

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