

The Mobility and Kinetics of Solutes in Ni-Al-Cr Superalloys: An Atomic Scale Study by Kinetic Monte Carlo Simulations

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- ◆ The **diffusivities** of **Al or Cr solute** atoms and **clusters** of these atoms in Ni are studied utilizing kinetic Monte Carlo simulations at 600°C.
- ◆ Al, Cr or Al-Cr **n-mer clusters** are more **mobile** than Al or Cr **monomers** up to $n = 5$ for Al, $n = 3$ for Cr, which is relevant to the **cluster-diffusion-coagulation** mechanism for **coarsening**.
- ◆ The **precipitates** that coagulate and coalesce are connected by **necks** that preserve the **chemical sequence** of an ordered $L1_2$ structure between precipitates, such that an **anti-phase boundary** is not introduced because it is energetically unfavorable.
- ◆ **Necks** between precipitates are most likely the result of **small solute clusters** attaching themselves to precipitates that are initially close to a **[110]** direction. The clusters form a **bridge** between precipitates.
- ◆ KMC simulations demonstrate that **necks exist** between precipitates when the **vacancy-solute** binding energies are **present** and **absent** when they are **zero**.

