

Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Medium-range order in $\text{Al}_{90}\text{Sm}_{10}$ liquids revealed by a pre-peak in the structure factor FENG ZHANG, YANG SUN, XIAO-WEI FANG, MATTHEW KRAMER, MIKHAIL MENDELEV, RYAN OTT, CAI-ZHUANG WANG, KAI-MING HO, Ames Laboratory — Aluminum (Al) alloyed with about 10 at.% rare-earth metals such as samarium (Sm) can display promising mechanical properties upon rapid quenching from the liquid state. Knowledge about the structure of the liquid phase is an important starting point for understanding the profound phase selection during the rapid solidification process, which plays a key role in materials performance. We have performed ab-initio molecular dynamics (AIMD) calculations on the liquid $\text{Al}_{90}\text{Sm}_{10}$ system with 500 atoms per unit cell at $T = 1300$ K, which is well above the melting temperature of the system. The AIMD simulations show that the liquid system develops a medium-range order by segregating into nanometer-sized regions with different atomic compositions. This segregation ultimately gives rise to a distinct pre-peak in the structure factor observed both in experiments and in AIMD calculations. Our results are in good agreement with experimental measurements using three-dimensional atom probe on the amorphous $\text{Al}_{90}\text{Sm}_{10}$ structure rapidly quenched from the liquid state.

Feng Zhang
Ames Laboratory

Date submitted: 15 Nov 2013

Electronic form version 1.4