doi:10.1017/S1431927613006661
Microsc. Microanal. 19 (Suppl 2), 2013

A Level Set Evaporation Model for Heterogeneous Atom Probe Tip

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With the development of local electrode atom probe tomography (LEAP), the materials systems feasible for atomic structure determination has expanded from predominantly metals to include heterogeneous materials with complex structure and compositions. This makes the 3D atomic structure determination possible for most energy materials in battery, fuel cell, semiconductor, and nuclear applications. Atom probe tomography (APT) has been utilized to study multiphase materials with segregation and interface problems [1]. The unique and quantitative information retrieved from APT can provide a foundation for the study of kinetic pathways, nanoscale composition mapping, multilayer interfacial segregation, dislocations and grain boundaries. However, a new challenge surfaces when the materials systems expand into heterogeneous materials: the traditional structure reconstruction introduces false magnification and large artifacts due to the underlying assumption of uniform and isotropic evaporation.

Traditional image reconstruction from the ion graphs in detectors to 3D structure is limited to the assumption of homogeneous structure and evaporation rate for different components. However, it is not the case in a heterogeneous system consisting of phases with different evaporation behavior. For most complex materials systems, these traditional methods will create global distortions, trajectory overlap, and localized false magnification. To take full advantage of the high resolution inherited in atomic probe tomography, a new efficient and accurate tip evaporation simulation model is crucial for next generation atomic structure reconstruction software [2-6].

In our approach, a level set based evaporation model is developed to simulate the evolution of tip surface morphology during the evaporation of multi-layered heterogeneous materials. Current evaporation models for APT widely utilize the approach of finite element method, which is computational expensive and lack of subgrid scale accuracy, especially when the interface curvature and normal are involved in the calculation for atomic evaporation. Our preliminary results demonstrated an increase of efficiency with no sacrifice of accuracy comparing with the standard FE method.

Level set method is originally introduced for solving multiphase flow problems involving dynamic and complex interface evolution between two phases. Historically these “moving boundary and/or interface” problems have been very challenging from a computational point of view. Level set method [7] is based on the tracking or capturing of sharp interfaces, while complex geometries and morphology changes can be handled efficiently. It has been applied to interface tracking in the areas of computational fluid dynamics and fracture propagation in the framework of extended finite element method. For evaporation simulation, we use level set method to investigate the dynamic evolution of the interface between two distinct phases, namely the vacuum phase and the material phases. A continuous level set function $\phi(\boldsymbol{x})$, is introduced which is positive in vacuum and negative in the materials. The zero-level of the level set function denotes the exact position of the interface between vacuum and material phases, i.e.

$$\Gamma = \{x{:}\phi(x) = 0 | x \in \Omega\},$$

where level set function ϕ is defined as the signed distance to the interface. By this means, the interface can be implicitly represented by the zero-level of level set field. The evolution of entire level set field is numerically computed based on hyperbolic conservation laws. Due to the advantage of the level set

method, our model can handle problems where the interface moving velocity is sensitive to the local geometry such as curvature and normal direction, as well as the evaporation physics of heterogeneous materials across the interface.

In our preliminary simulations, a level set model has been applied to tip samples with two different geometries. The first one is a composite containing of a spherical particle with high evaporation field strength embedded in a matrix material with low evaporation field strength, as shown in Figure 1(a). Figure 1(b) shows a snapshot of the tip shape after evaporation demonstrating the stick out of the material with high evaporation strength. The second example is a bilayered composite with low evaporation field strength phase deposited on top of a high evaporation filed strength substrate. The tip shapes at the earlier and later stages of the evaporation simulation are illustrated in Figure 2. In contrast to the standard FEM model, the level set model improves computational efficiency and provides a smoother interface between two phases due to the inherent subgrid accuracy.

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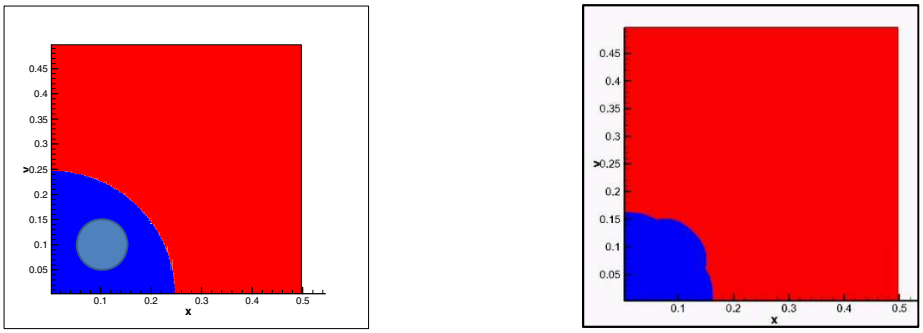
The authors acknowledge the funding support from the LDRD-funded Chemical Imaging Initiative at Pacific Northwest National Laboratory, operated for the U.S. Department of Energy by Battelle under contract DE-AC06-76RL01830.



(a) (b)

Figure 1. Tip shape evolution of a composite with a spherical particle simulated by level set method at (a) the beginning and (b) the final stages

Figure 2. Tip shape evolution of layered structure composite with low evaporation field strength layer on high evaporation field strength substrate, simulated at (a) earlier and (b) later stages.

https://doi.org/10.1017/S1431927613006661 Published online by Cambridge University Press