THERMOPHYSICAL PROPERTIES OF INTRINSIC POINT DEFECTS IN CRYSTALLINE SILICON

Talid Sinno
Department of Chemical Engineering
University of Pennsylvania
Philadelphia, PA 19104-6393, USA

The study of intrinsic point defect dynamics during silicon crystal growth and wafer processing has had a long and rich history. Despite an enormous body of work on the subject, quantitatively robust models based on the dynamics of point defects in silicon have yet to be developed. A major limitation is the accuracy of estimates for the thermophysical properties of point defects, namely diffusion coefficients, equilibrium concentrations, and reaction kinetics. An overview is presented of the various theoretical and experimental approaches taken for determining these properties. In particular, the predictions for point defect properties obtained from metal (Zn [1], Pt, and Au [2]) and dopant (Group III and V) diffusion during wafer thermal annealing are compared to those obtained using single crystal ingot growth. Lastly, the predictions of model fitted thermophysical properties are discussed in the context of atomistic simulations. Results from *Ab initio*, tight-binding, and empirical potential simulations are considered.

A detailed presentation is given of recent work aimed at using the Czochralski (CZ) crystal growth system to extract high temperature self-interstitial and vacancy thermophysical properties. An example of the experimental data used for this study is shown in Fig. 1 [3], in which the interstitial-vacancy boundary (IVB) and the Oxidation-Induced Stacking-Fault Ring (OSF-R) [4] can be delineated. The dependence of these features on variations in the crystal growth rate provides a sensitive method for probing intrinsic point defect properties. It is shown that a fully transient analysis is necessary to capture accurately the behavior of the OSF-R and IVB when the crystal growth rate is varied during growth. The predictions of the transient model fitting are compared to the results of previous steady state analyses of OSF-R dynamics [5,6].

A global optimization approach based on Simulated Annealing (SA) [7] is developed and used to compare systematically the predictions of computer models with experimental measurements. While the convergence to a global optimum of the SA method cannot be guaranteed, it is necessary for model fitting because of the presence of multiple parameter sets that are locally valid. The latter fact is most likely an important factor for the wide range of reported poinjt defect properties in the literature. Results from fitting point defect properties to a single crystal growth experiment are shown in Figure 2. The thermophysical properties that led to this fit also were required to satisfy currently accepted estimates [8] for the vacancy and interstitial self-diffusion contributions. The SA approach also is shown to be suitable for fitting simultaneously the data from several experimental sources. In this way, the uncertainty associated with model fitting is reduced by increasing the number of features that must be reproduced with a single set of point defect thermophysical properties.

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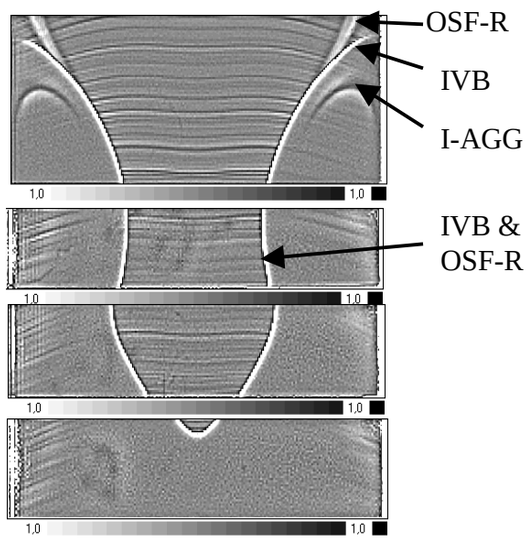

Figure 1: Axial cross-section X-ray topograph of a CZ ingot showing (i) the OSF-ring (OSF-R), (ii) the interstitial/vacancy boundary (IVB), and (iii) the boundary for the region of interstitial dislocation-loop formation (I-AGG).

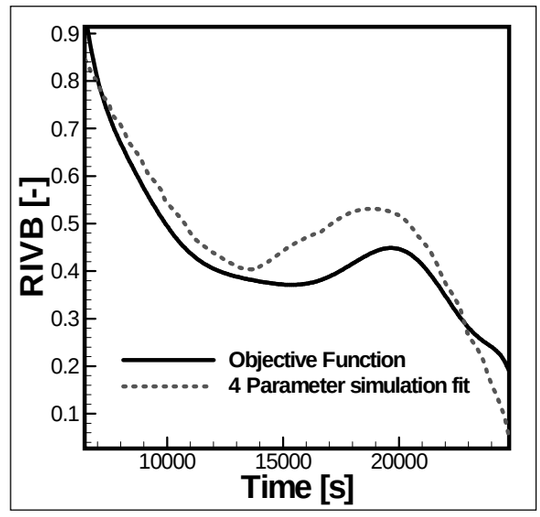

Figure 2: Comparison of the best-fit (dashed line) and experimentally measured positions (solid line) of the IVB.