Simplified Two-Dimensional Quantification of the Microdefect Distributions in Silicon Crystals Grown by Czochralski Process

[a]Milind S. Kulkarni and [b]Vladimir V. Voronkov
[a]MEMC Electronic Materials, St. Peters, MO 63376, USA
[b]MEMC Electronic Materials, 39012 Merano BZ, Italy

The continuously shrinking size of the modern microelectronic device imposes challenging restrictions on the quality of the silicon substrate, which is essentially determined by the size and the distribution of the precipitates known as microdefects. Most of the microdefects formed in a growing silicon crystal, in the Czochralski (CZ) process, are the agglomerates of intrinsic point defects of silicon – vacancies and self-interstitials. The quantification of the microdefect distribution involves a solution of complex equations that must be numerically solved. Traditionally, microdefect dynamics is captured by decoupling the initial incorporation of the point defects, which describes the establishment of a concentration field of the dominant point defects beyond a characteristic distance from the melt/crystal interface and the subsequent formation of the microdefects.[1,2] Another approach is a rigorous numerical simulation based on the Fokker-Planck approximations.[3] The former approach cannot accurately capture the microdefect distribution, because the concentration field of the point defects is actually affected by their diffusion toward the microdefects. The latter approach is numerically expensive.

In any region of a growing CZ crystal, moving at the crystal pull-rate, there exists a distribution of the microdefects of varying sizes formed at different instants. The microdefects can be reasonably approximated as spherical clusters.[1-4] The diffusion-limited flux of the dominant point defects to the clusters is given by the following equation:

$$Q_j = 4\pi D_j \left(C_j - C_{j,e}\right)\int_0^t R_{cl,j}(\tau,t) J_{cl,j}(\tau) d\tau$$

where the subscript j refers to the point defect species, cl – to the clusters, and e – to the equilibrium conditions; $R(\tau,t)$ is the radius of the clusters present at the region at time *t* but formed previously, at elapsed time τ, $J(\tau)$ is the nucleation rate of the point defects, and C is the point defect concentration. To capture microdefect dynamics, the concentration field (C) and the cluster size distribution at all regions of a crystal are required. Hence, the solution of the governing equations describing microdefect dynamics is computationally expensive.[4] This set of equations can be greatly simplified by replacing the averaged cluster radius (that actually enters the above equation for Q_j) with the square root of the average of the squared cluster radius, $\Re$. The cluster population is thus represented just by the total cluster density *N* and the auxiliary variable U (that is equal to the total cluster surface area divided by 4π):

$$\Re_{cl,j}^2 = \int_0^t R_{cl,j}^2(\tau,t) J_{cl,j}(\tau) d\tau \Big/ \int_0^t J_{cl,j}(\tau) d\tau$$

$$N_{cl,j} = \int_0^t J_{cl,j}(\tau) d\tau; \quad U_j = \int_0^t R_{cl,j}^2(\tau,t) J_{cl,j}(\tau) d\tau$$

Using this formulation, the point defect consumption rate by the clusters can be rewritten as

$$Q_j = 4\pi D_j \left(C_j - C_{j,e}\right)\left(U_j N_{cl,j}\right)^{1/2}$$

The kinetic equation for the variable *U* follows from the cluster growth kinetics, and *N* changes because of the nucleation:

$$\frac{\partial U_j}{\partial t} = \frac{2}{\psi} D_j \left(C_j - C_{j,e}\right) N_{cl,j}; \quad \frac{\partial N_{cl,j}}{\partial t} = J_{cl,j}(t)$$

where ψ is the density of the point defects in the clusters. Thus, microdefect dynamics can be described by a set of differential equations for C, N, and U. The new formulation captures the representative average size of the clusters and does not require the knowledge of the history of formation and growth of the clusters.

The microdefect distributions in various CZ crystals grown using time-dependent pull-rates were predicted by the developed model. The model predictions agree well with the experimentally observed microdefect distributions. The new model considerably reduces the computational complexity and can be reliably applied in the development of new processes.

References:

1. V. V. Voronkov, *J. Crystal Growth*, **59**, 625 (1982).
2. V. V. Voronkov and R. Falster, *J. Cryst. Growth*, **194**, 76 (1998).
3. T. Sinno and R. A. Brown, *J. Electrochem. Soc.*, **146**, 2300 (1999).
4. M. S. Kulkarni, V. V. Voronkov and R. J. Falster, in *High Purity Silicon VII*, C. L. Claeys, M. Watanabe, P. Rai-Choudhury, and P. Stallhofer, Editors, PV 2002-20, p27, The Electrochemical Society Proceedings Series, , Pennington, NJ (2002).

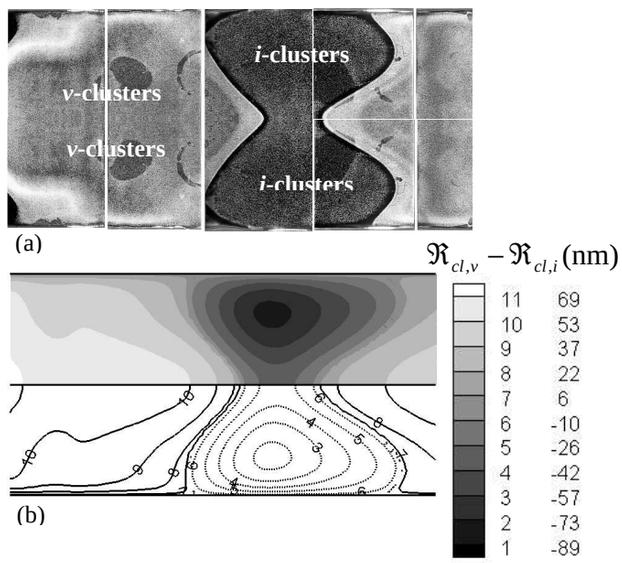

Figure 1. (a) The experimentally observed microdefect distribution in a CZ crystal, where *i*-clusters represent interstitial agglomerates and *v*-clusters represent vacancy agglomerates (voids). (b) The model-predicted microdefect distribution is shown through the distribution of the difference in the radius of *v*-clusters and the radius of *i*-clusters. The positive numbers indicate the *v*-cluster size and absolute values of the negative numbers indicate the *i*-cluster size. Clusters of different type (*i*, and *v*) do not coexist.