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Dislocation Generation by Thermal Stresses in Si: Modeling and Experiments

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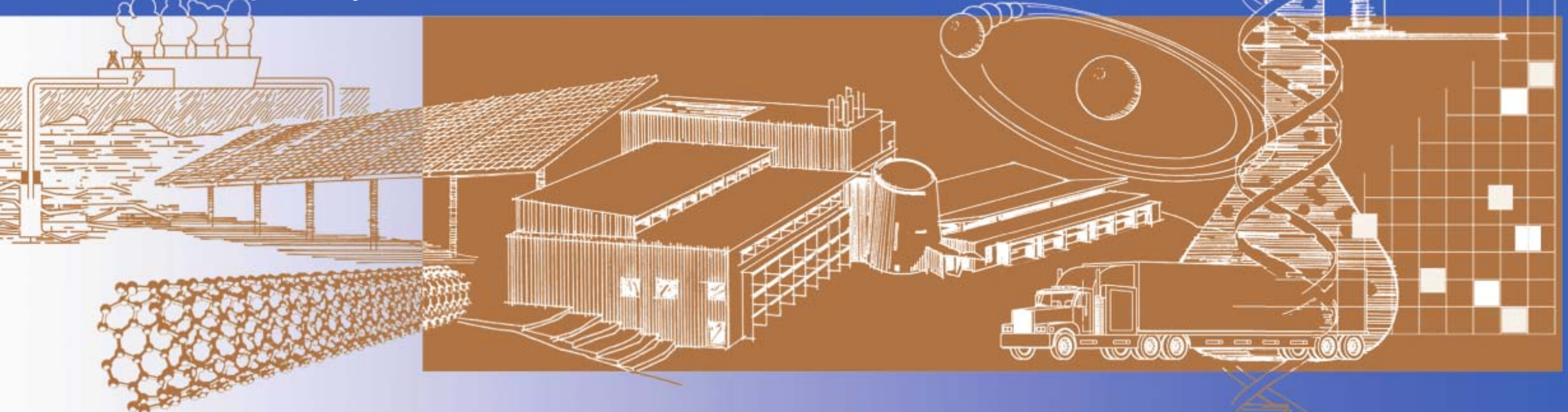

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Dislocation Generation by Thermal Stresses in Si: Modeling and Experiments

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ABSTRACT

We developed a finite-element modeling program to predict the thermally generated dislocation distribution in a wafer. This model uses measured parameters that are determined from generating dislocations under a known optical flux.

1. Objectives

Dislocations in Si increase carrier recombination. They also interact with impurities, leading to additional recombination and impurity precipitation. Both these mechanisms result in severe degradation in solar cell performance. In fact, in many low-cost solar cells, the limitation in the cell performance is produced by the presence of dislocations. One solution to this problem is to significantly lower the dislocation density and minimize clustering of defects. This approach requires detailed thermo-mechanical modeling that can predict defect generation during crystal growth and can arrive at suitable dynamic thermal profiles, which can significantly lower defect densities.

Our objective is to develop a thermo-mechanical model that can accurately predict dislocation distribution corresponding to a given temperature profile for both single- and multicrystalline silicon (mc-Si) crystal growth. We will then use this model to predict temperature distributions that can minimize the dislocations in various types of crystal growth.

2. Technical Approach

Thermo-mechanical modeling has been successfully used to predict buckling, and residual stresses during crystal growth [1-3]. However, it has only had moderate success for predicting dislocation distributions in rapidly grown materials, such as cast and ribbon mc-Si. One major problem is that the current models use a simplified relationship between plastic deformation and the resultant dislocation density. This relationship is based on dislocation multiplication by a uniform shear strain, and requires an "initial" dislocation density—a parameter that cannot be determined. To overcome this limitation, we are developing a theoretical model that will use input parameters that can be experimentally determined by measuring the dislocation pattern produced in a wafer by a known thermal profile.

We are performing both experimental and theoretical studies to establish a relationship between the thermal stresses and resultant dislocation distributions. Experiments involve subjecting single- and mc-Si wafers (typically 4.5 in. x 4.5 in.) to predetermined thermal stresses by exposing them to known optical flux distributions (see Fig. 1). A commercial instrument, GT-PVSCAN, is used to measure the resultant dislocation distributions. These distributions are correlated with the theoretical stress distributions calculated by finite-element (FE) modeling, which includes appropriate boundary conditions for single- and mc-Si. Experimental results establish changes in the dislocation distribution as a function of time, temperature, and stress distributions.

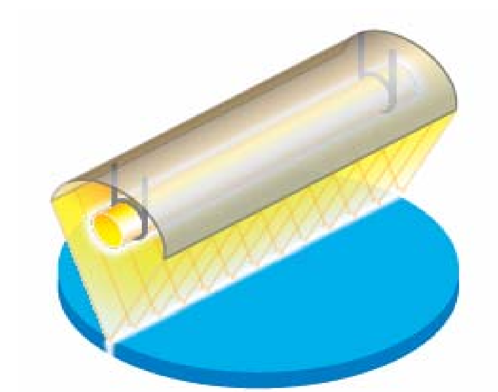

Fig. 1. Wafer processing using a linear infrared heater.

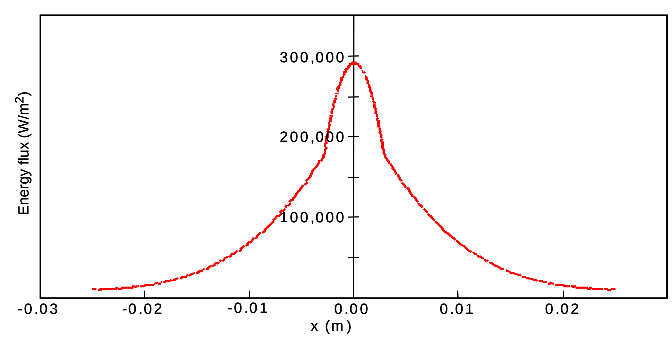

Fig. 2. Distribution of energy on the wafer surface along the line perpendicular to the heater axis.

3. Results and Accomplishments

Figure 2 shows a typical flux distribution used to generate dislocations in a Si wafer. Figure 3 shows a temperature distribution calculated for a flux distribution of Fig. 2. Because of the symmetry, only one-quarter of the wafer is shown. Maximum stress occurs along the X = 0 axis. This temperature distribution produces stress distributions that can be calculated for elastic and plastic regimes.

Dislocations were generated on single-crystal wafers of two orientations, (100) and (111). Figure 4 shows a dislocation map of a (100) sample produced by illuminating the wafer with a flux corresponding to that shown in Fig. 2. The dislocation map was generated by a GT-PVSCAN. Based on these results, the maximum density of dislocations is found to be about $4.10^6/cm^2$. We examined the directions of dislocation propagations. Figure 4 also shows photographs of the defect-etched sample, with dislocation formation along the slip directions. One can also see dislocation network formation caused by slip on different (111) planes.

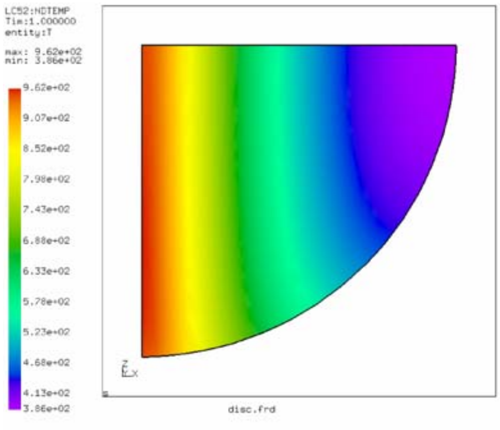

Fig. 3. Calculated temperature distribution corresponding to the flux profile of Fig. 2. Because of the symmetry, only a quarter of the wafer is shown.

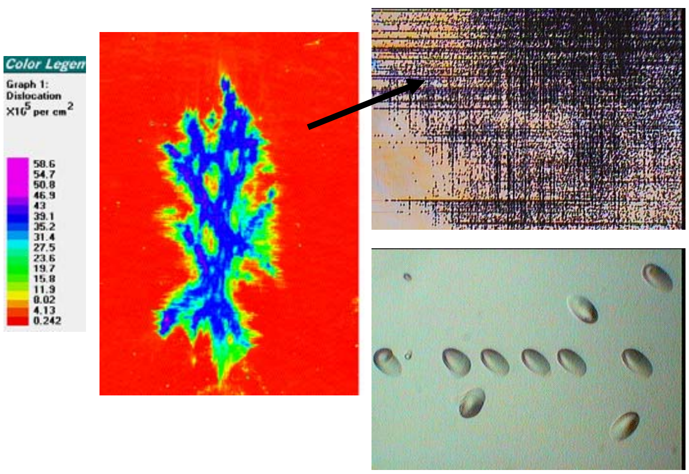

Fig. 4. Dislocation density distribution produced in a (100)-oriented single-crystal wafer by the flux distribution of Fig. 2. Also shown is etch-pit distributions with dislocation generation along slip directions.

Figure 3 shows very high temperature gradients between the center (962ºC) and the cold edge (386ºC) of the wafer. Note that the temperature distribution observed in Fig. 3 was generated by only one linear heater that focuses energy along the line going through the center of the wafer (x=0). For the temperature profile illustrated in Fig. 3, stress distributions were also computed for purely elastic and elasto-plastic models. We observed that the stresses concentrate along the central line (x=0) and that the highest value is located in the proximity of the wafer edge. It is important to note that both the highest stresses and highest temperatures were found in the same region of the wafer. Because the yield stress is inversely proportional to the temperature, one would expect the material to deform plastically in this region. The results from the elasto-plastic model clearly indicate that the magnitude of stress in the hottest parts of the wafer decreased significantly when compared to the elastic case. Obviously, this effect was attributed to plastic yielding. The regions where the material yielded are illustrated in Fig. 5, which depicts the distribution of the plastic strain on the wafer surface. Clearly, there is a strong correlation between the location of the nonzero plastic stain in the numerical results and the location of the plastic zone in the experimental images.

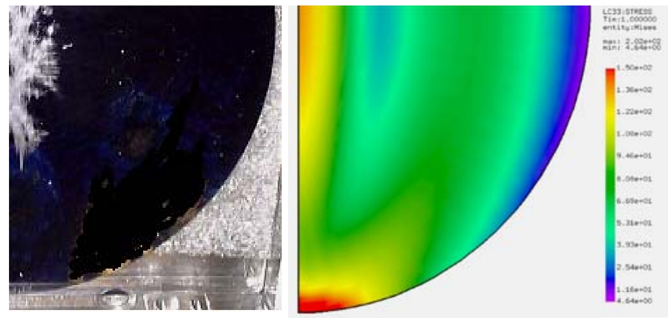

Fig. 5. A comparison of the dislocation formation (left) and the calculated plastic deformation (right).

4. Conclusions

We observed an excellent correlation between the actual dislocation distribution and the calculated plastic strain. Further studies are under way to determine dislocation evolution as a function of time and temperature distribution (stress), and to include derived parameters into the theoretical model. Our studies have also shown that there is a strong dependence of yield stress on the wafer orientation. For example, under the thermal stresses produced by the flux distribution of Fig. 2, (111) wafers do not result in any dislocation generation. Thus, the yield stress for (111) wafer is considerably higher than for (100). This orientation dependence of yield stress has an important bearing on the formation of defect clusters in mc-Si used for solar cells. The physical mechanism associated with this effect is that when thermal stress exceeds the critical shear stress in grains of a particular preferred orientation (those with slip directions along the shear), they locally yield and relieve stress by local generation of dislocations. This mechanism leads to “clustering” of dislocations, which produce severe degradation of solar cell performance [4].

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