ScienceDirect

Materials Science and Engineering: B

Volumes 159–160, 15 March 2009, Pages 248-252

As-grown iron precipitates and gettering in multicrystalline silicon

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Received 2 May 2008, Revised 21 October 2008, Accepted 30 October 2008, Available online 3 December 2008.

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https://doi.org/10.1016/j.mseb.2008.10.053

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Abstract

We report here the results of a theoretical study concerning the iron precipitation in multicrystalline silicon during crystal growth and its implications on phosphorus gettering. In our model the average size and density of iron precipitates in the final structure depends on the growth method, initial iron concentration and the density of possible heterogeneous precipitation sites. With the same model we can simulate phosphorus diffusion gettering (PDG) of iron in cast multicrystalline silicon by using the iron precipitate size distribution obtained from crystal growth simulations as initial condition for gettering.

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Introduction

Multicrystalline silicon contains high concentrations of iron, typically in the range of 10^{14} to $10^{16}\,cm^{-3}$. Iron is mostly precipitated at grain boundaries and at structural defects, and approximately only 10^{12} to $10^{13}\,cm^{-3}$ of iron remains in interstitial sites after crystal growth [1], [2]. Diffusion of high concentration of phosphorus (P) is a well-known gettering technique for removing iron in silicon technology and it is a crucial part of a high efficiency solar cell process. Theoretical results of gettering of precipitated iron in multicrystalline silicon are presented in several papers [3], [4]. Usually it is assumed that all iron is precipitated to some density of iron precipitates and a diffusion limited growth law is used to simulate the time evolution of average size of iron precipitates.

In this paper we study theoretically the iron precipitation process during multicrystalline silicon growth using the heterogeneous precipitation model presented in Refs. [5], [6], originally developed for single crystal silicon. Particularly, we consider into details the cooling rate, which depends on the crystal growth method, and its effect on the size distribution of as-grown iron precipitates and the efficiency of phosphorus diffusion gettering (PDG).

Section snippets

Modeling of heterogeneous iron precipitation and phosphorus gettering

In Refs. [5], [6] we have presented a lumped model for heterogeneous precipitation of iron in single crystal silicon, which has been used to model internal gettering. The model assumes that the heterogeneous precipitation sites that already contain some iron are more attractive gettering sites than the ones with no iron, simply because of a lower chemical

potential of iron in large precipitates. This assumption, together with the Fokker-Planck Equation (FPE) used to simulate the cluster…

As-grown iron precipitates

At the moment several crystal growth techniques are in use, such as String Ribbon (SR), edge-defined film-fed (EFG), and directionally solidified ingot growth. SR and EFG growth techniques have faster cooling rates after crystallization than ingot growth [1]. Thus, we made a series of simulations assuming either fast (45 °C/min) or slow (1 °C/min) cooling during crystal growth [16]. The initial iron concentration and the density of heterogeneous precipitation sites were varied between 10^{14} to 10^{15}…

Conclusions

We have made a series of simulations of iron precipitation during multicrystalline silicon growth. We have observed that we can interpret in a reasonable way the published experimental results of iron silicide precipitates although for simplification we have used a point-size simulation for iron precipitation during multicrystalline silicon growth. We have shown that PDG of iron can be simulated in cast multicrystalline silicon by combining the initial conditions from point-size crystal growth…

Acknowledgements

The authors acknowledge the financial support from the Finnish National Technology Agency, Academy of Finland, Okmetic Oyj, Endeas Oy, Semilab Inc. and VTI Technologies Oy.…

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> *Citation Excerpt :*
> ...The interaction of metal precipitates with gettering sites, which results in an apparent change of local solubility, is modelled by a fitting parameter. Haarahiltunen's model was first applied to the internal gettering of Fe by oxide precipitates in Cz-Si [61,62], and later extended to gettering of Fe by extended defects in mc-Si [63], damage in boron [64,65] and phosphorus [21] ion implanted regions, and surface precipitation in heavily boron doped Si [66]. Zhang et al.'s experimental data of Fe precipitate dissolution from oxide precipitates [56] could be simulated using Haarahiltunen et al.'s model, without the need to explicitly include a binding energy between precipitates and gettering sites [62]....

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