

Analysis of the mechanism of diffusion limited oxygen precipitation in Cz-silicon

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Abstract

We develop models for diffusion limited oxygen precipitation. We analyze the specific boundary conditions for the diffusion equation and we study the validity of the synchronic evolution of the precipitation cells. The combined model describes the simultaneous evolution of growing and dissolving precipitates.

1. Introduction

The control of oxygen precipitation in silicon is a vital problem in VLSI-ULSI technology. The evolution of oxygen precipitates has been an intensively studied subject in scientific literature, but there still are unclarified aspects.

The precipitation process in solids was first studied in relation to steel metallurgy, the first models being intended to explain the carbon precipitation in steel [1,2]. The equation which describes this process was given in 1950 by Wert [1]. His hypotheses are the supports for a more rigorous development of the diffusion controlled precipitation model done by Ham [2] in 1958. This theory is based on the existence of analytical solutions of Wert's equation which are obtained as a series with a dominant first term.

In this paper we intend to analyze and explain some of the hypotheses of the earlier theories, and to suggest new developments of the theory of oxygen evolution in silicon.

2. Development of the models

In a real silicon crystal the oxygen precipitates are uniform and randomly distributed in space, and the sizes of the precipitates are arbitrary. The crystal may be divided into cells of arbitrary shape and size, in such a way that each cell contains one precipitate and only one. We accept, as an initial approach, that the precipitates are all growing, or are all dissolving.

In the bulk of the crystal the oxygen diffusion process can be described by the formula:

$$\frac{\partial C}{\partial t} = D \Delta C, \quad (1)$$

with the initial condition

$$C(r, t) = C_0, \quad (2)$$

where D is the diffusion coefficient, and C the concentration of interstitial oxygen. The boundary conditions are given generally at the surface of a precipitate by

$$-D \left. \frac{\partial C}{\partial n} \right|_s = \beta (C - C_s), \quad (3)$$

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