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Mesures de diffusion dans SiO_2 et dans SiC

Hartmut Bracht
Kirsten Sunder
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Jeudi 5 mars 2009 à 10h

Horaire anticipé, Séminaire en deux parties
pause café entre les deux parties

N.B : ***Les visiteurs de nationalité étrangère hors Union Européenne sont priés de bien vouloir avertir impérativement 3 semaines à l'avance – les visiteurs de l'Union Européenne 1 ou 2 jours avant le séminaire – le Secrétariat du Service de leur entrée sur le Centre :***
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Part 1: Oxygen and silicon diffusion in amorphous silica

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Amorphous silica (SiO_2) is an important material for electronic applications. Silica doped with alkali and alkaline-earth oxides are even more widely spread as e.g. window glasses. The addition of alkali and alkaline-earth oxides leads to the formation of non-bridging oxygen. The induced microstructural changes give rise to lower glass transition temperatures. As a consequence also the mobility of the network formers oxygen (O) and silicon (Si) should be altered. In order to study the impact of alkali and alkaline-earth oxides on the network dynamic we first consider the diffusion of O and Si in pure silica. Several experiments and calculations on the diffusion of the network formers were performed during the past twenty five years. The diffusion coefficients reported in the literature spread over several orders of magnitude indicating major differences in the sample preparation and ambient conditions realized in the diffusion experiments.

On the basis of a point defect model we can explain most experimental results reported in the literature. Our model considers defects for O- and Si-rich conditions that are supported by first-principles calculations of Roma et al. (Defect and Diffusion Forum 258-260, p.542 (2006)). In addition, the impact of a moving SiO_2/Si interface on the O and Si diffusion is taken into account. Numerical simulations based on our point defect model provide accurate fits to the experimental profiles given in the literature and to those measured within the scope of this work. The model parameters determined from the numerical calculations are discussed and compared to literature data. First results on the impact of doping with alkali and alkaline-earth oxides on the mobility of the network formers are presented but additional studies are still necessary to discover general trends.

Part 2: Interrelation between self- and dopant diffusion in silicon carbide

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Silicon carbide (SiC) is a semiconductor with a wide band gap energy. The distinguished chemical and radiation resistance of SiC compared to other semiconductors and its excellent electronic properties make SiC an ideal material for high-power, high-temperature, and high-frequency electronic applications.

Selective doping of SiC is generally achieved by ion implantation and subsequent annealing to activate the dopant. Ion implantation introduces vacancies (V) and self-interstitials (I) on both sublattices whose concentrations can significantly exceed their concentrations under thermal equilibrium. As a consequence, the diffusion of dopants can be strongly affected by implantation-induced defects during the earlier stages of a thermal treatment until the implantation damage is recovered. In order to understand dopant diffusion in SiC, in particular after ion implantation, the dopant diffusion mechanisms and the nature of the point defects involved are of fundamental and technological significance.

In this work we present experiments on C and Si self-diffusion in isotopically controlled 4H-$^{28}Si^{12}C/^{nat}SiC$ heterostructures at temperatures between 2000℃ and 2450℃. In order to gain information on the native point defects that mediate self-diffusion we also investigated the diffusion of boron (B) and phosphorous (P) in SiC. Modelling the diffusion and reactions of dopants in SiC by means of continuum theoretical (CT) calculations provide information about the nature of the point defects, their charge states, and their diffusion activation enthalpy. The interrelation between self- and dopant diffusion reveals that doubly positively charged C interstitials and singly charged Si vacancies mediate C and Si diffusion in SiC, respectively. The relevance of the point defects assumed in our CT calculations is supported by recent ab initio simulations.