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Theoretical study of A→B structure transition in thin epitaxial CaF_2 films on Si(111) surface

A.F.Oshkalo, O.A.Zhikol, O.V.Shishkin, A.G.Fedorov, A.V.Belenchuk[*]*, O.V.Prezhdo*[**]

Institute for Single Crystals, National Academy of Sciences of Ukraine,
60 Lenin Ave., 61001 Kharkiv, Ukraine
[*]Institute for Applied Physics, Academy of Sciences of Moldova,
Kishinev, Moldova
[**]Chair for Chemistry, Washington University, Seattle, U.S.A.

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From two models proposed for thin film CaF_2/Si(111) structure basing on experimental results, the energetically favorable one has been chosen using atom-atom potential calculations. Basing on the calculated mean silicon atom-fluorine ion interaction energy for particle normal vibrations at 473 K and 673 K, the energy gain due to A→B structure transition accompanying the substrate temperature elevation has been demonstrated. The A→B film structure transition is concluded to be caused by increasing amplitudes of particle vibrations due to temperature increase.

Из двух предложенных экспериментальным методом исследования моделей структуры переходной зоны пленки и подложки в тонких пленках CaF_2/Si(111) выбрана наиболее энергетически выгодная в рамках метода атом-атомных потенциалов. На основании рассчитанной средней энергии взаимодействия между атомами кремния и ионами фтора при колебаниях частиц для 473 K и 673 K показана энергетическая выгодность перехода пленки структуры A в B при повышении температуры подложки. Сделан вывод о том, что причиной перехода пленки структуры A в B является увеличение амплитуд колебаний частиц с повышением температуры.

The epitaxial CaF_2 films on silicon surfaces are integral parts of many semiconductor devices, such as IR ones [1–5] and field transistors [6]. At present, it is just the (111) silicon surface that is recognized universally as the best substrate for growing nanostructures of that kind [1].

The CaF_2/Si(111) interface structure was studied using several experimental techniques. Two orientations of CaF_2 film being grown on Si(111) surface have been found to be possible [1], namely, the A one where the film has the same crystallographic orientation as the substrate and the B structure where the film is turned at 180° about the (111) axis, similar to the twinning in the crystals [1], see Fig.1. These two film types can coexist in samples as block structures in various ratios, depending on the growth conditions. In such cases, films grown under different conditions differ in the crystal structure perfection. In spite of that it is just the substrate perfection that is the decisive factor, the block film structure deteriorates its quality and thus the semiconductor device performance. Also, it was found in experiment that the A type films of less than 8 monolayers thickness transit into B ones as the substrate temperature increases [7].

The reasons for that transition as well as its mechanisms remain still unclear. The purpose of this work is to elucidate the causes of the A→B structure transition in