

Ultra-thin and thin CrSi films on Si(111): I. Formation and crystal structure

Nikolay G. Galkin,
Konstantin N. Galkin,
Oleg V. Kropachev,
Sergey A. Dotsenko
Dmitrii L. Goroshko,
Dmitri B. Migas,¹
Andrew B. Filonov,¹
Natalia V. Skorodumova,
Andrey V. Gerasimenko,
Anton K. Gutakovski.

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¹Belarusian State University of Informatics and Radioelectronics, 6 P. Brovki Street, Minsk, 220013, Belarus.

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Abstract: In this paper we present the results of ab initio calculations on the ground state of the CrSi bulk and experimental studies on the structure and morphology of thin and ultrathin CrSi films grown on Si(111) substrates. Even though CrSi is expected to crystallize in the simple cubic B20 structure (space group #198, P213), we show that the ground state of CrSi is monoclinic (space group #4, P21). According to

the calculated band structures monoclinic CrSi is a gapless semiconductor with holes as the main charge carriers and antiferromagnetic ordering, while cubic CrSi is a half-metal with ferromagnetic ordering. Ultra-thin CrSi films (3.19–4.31 nm) grown by the solid-phase epitaxy are indeed characterized by the monoclinic structure. For thin CrSi films (32–83 nm) fabricated by the molecular beam epitaxy, the coexistence of grains in the monoclinic and cubic phases is revealed in the films whereas the volume of these grains depends on the silicon to chromium flow ratio during the growth.

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