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

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SUPPLEMENTARY MATERIALS

Table T1 Fractional coordinates of atoms in the cubic (FM) and monoclinic (AFM) unit cells of CrSi

Monoclinic CrSi (#4, $P2_1$)			
	x	*y*	*z*
Cr1 (2*a*)	0.14335	0.13977	0.13295
Cr2 (2*a*)	0.64335	0.36023	0.86705
Si1 (2*a*)	0.85533	0.83303	0.85668
Si2 (2*a*)	0.35533	0.66697	0.14332
Cubic CrSi (#198, $P2_13$)			
Cr (4*a*)	0.13912	0.13912	0.13912
Si (4*a*)	0.84318	0.84318	0.84318

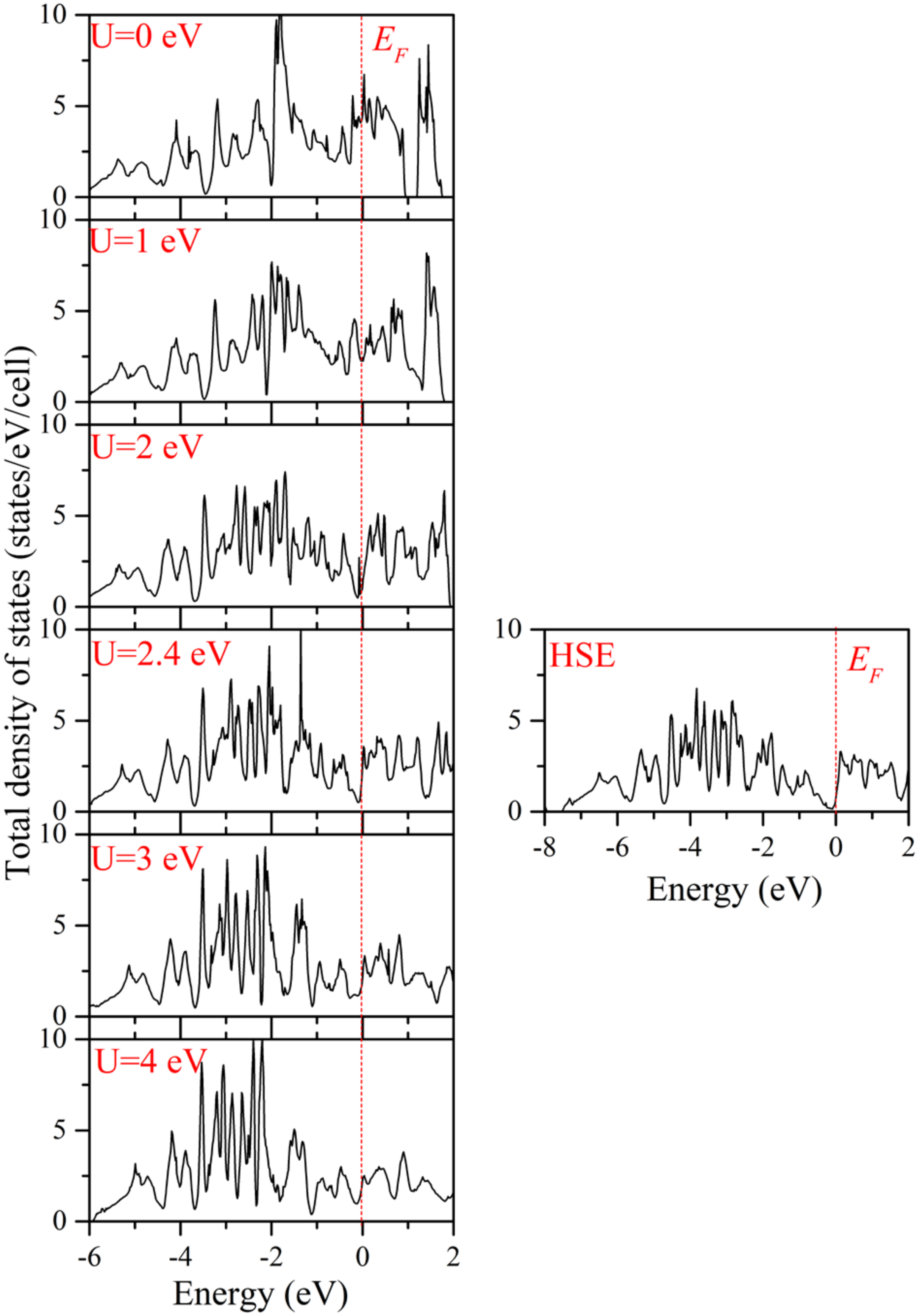

Figure S1. Comparison of the density of states of AFM monoclinic CrSi as calculated by GGA+U with different U (left panel) and HSE (right panel). Zero at the energy scale and the vertical dashed line correspond the Fermi energy.

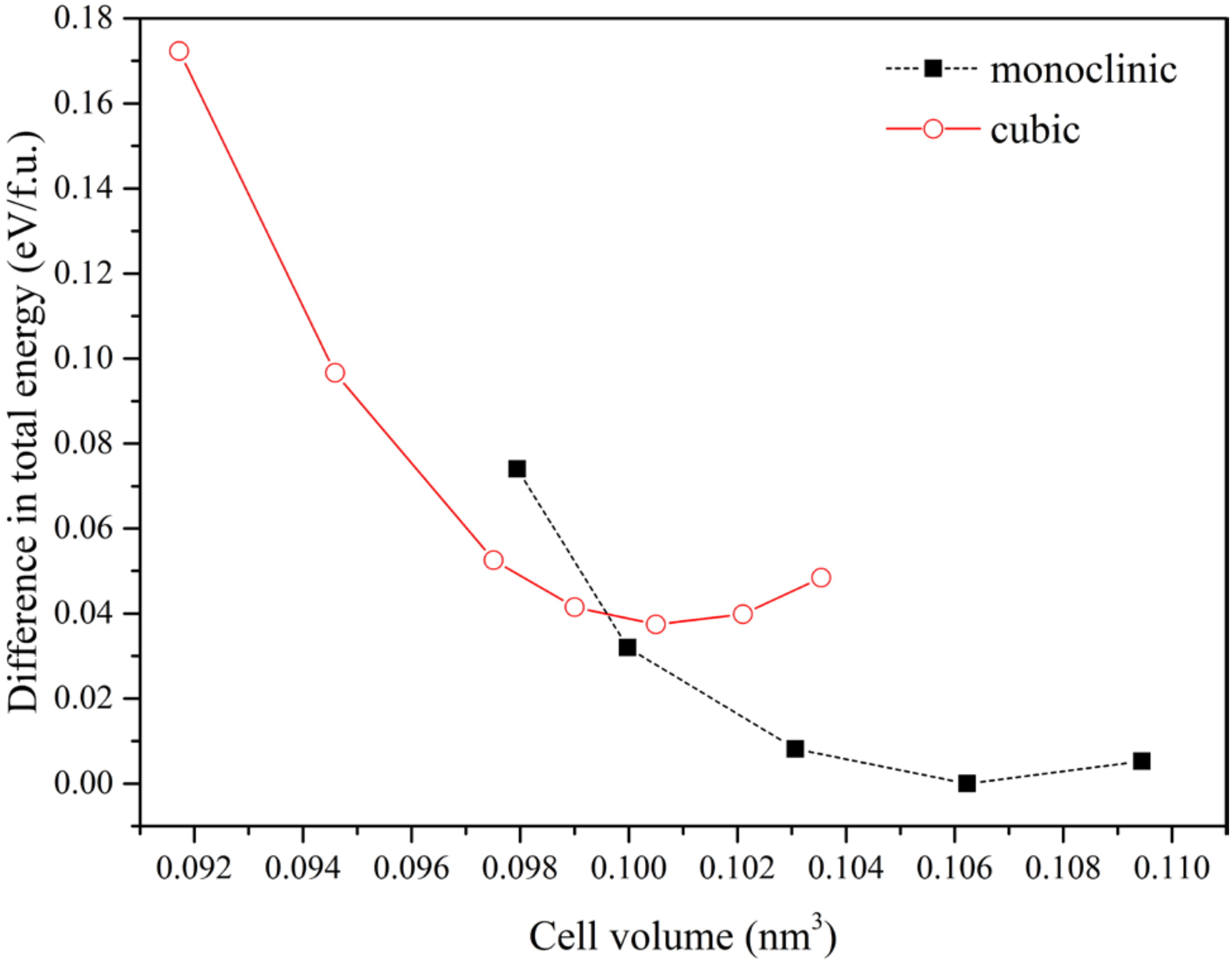

Figure S2. Difference in the total energies between the cubic and monoclinic CrSi phases under hydrostatic pressure as calculated by HSE. Lines connecting points are a guide to the eye.

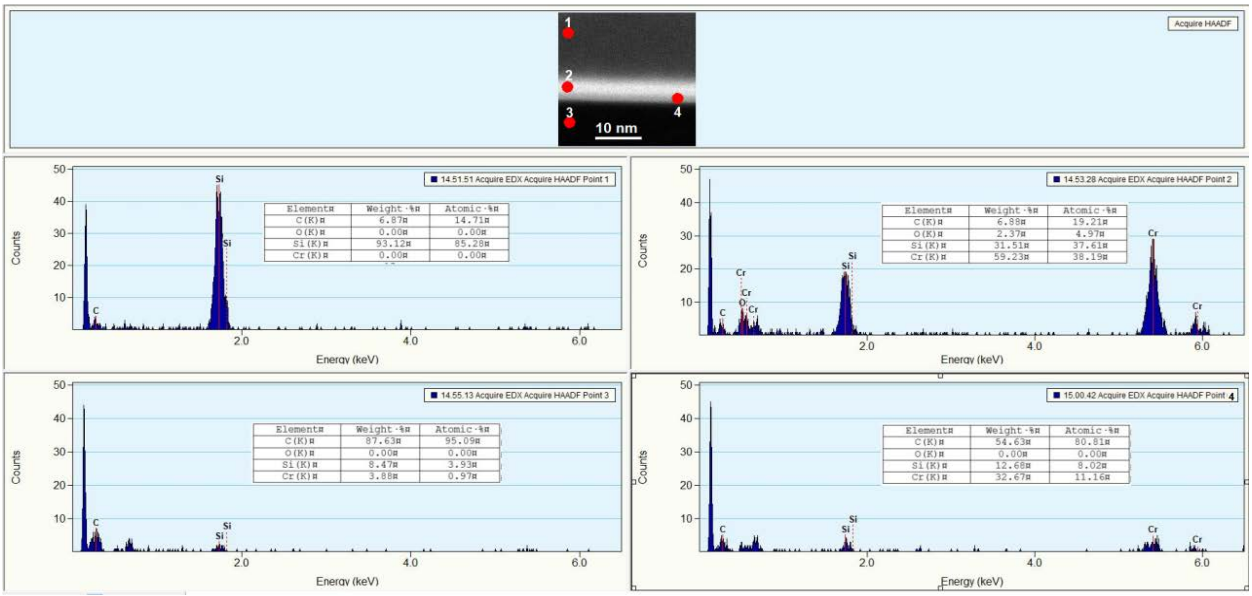

Figure S3. STEM HAADF image of a fragment of a cross section of the CrSi/Si(111) heterosystem (sample *A*, top) and EDX spectra for regions 1-4, marked with red circles: 1 – silicon substrate; 2 – CrSi film; 3 – compound; 4 – amorphous Cr layer.

The STEM HAADF and EDX data on the chemical content analysis for four regions in the cross section of CrSi/Si(111) are shown in Fig. S3 (the *A* sample, Fig. 4(a)). The semi-quantitative analysis of the regions 2 and 4 shows the chromium and silicon concentrations to be almost equal, confirming the chromium monosilicide formation. There is a carbon admixture in all the regions, which is an artifact of thin foil preparation with the use of ion etching. There is some oxygen concentration in the region 2 (the CrSi film) due to the oxygen adsorption on the foil surface after its preparation, and, at the same time, there is no oxygen at the film surface (the region 4). The chromium atoms are mainly contributed in this region, and the silicon contribution is about 1.4 times less, which corresponds to partial enrichment by chromium accounting for an averaging in the spectrum over the layer thickness at the point 4. That means that there is only an amorphous chromium layer (of 0.9 – 1.3 nm thick) on top of the monosilicide chromium layer (Fig. 4(a,c)), which contributed to a background in the FFT image (Fig. 4(d-g). It seemed that the annealing time was not enough to promote silicon atom diffusion from the substrate into the deposited chromium layer for the CrSi formation during the annealing. The same EDX data with the same results were obtained for the *B* sample (not shown here). Under the chromium thickness raised to 15.26 – 15.48 nm (the *C* and *D* samples, Table II) and the annealing temperature increased, silicon partially diffuses to the upper chromium layer, and it results in the formation of the CrSi grains. Two appropriate peaks at the angles of 44.79 – 44.91^{o} and 64.22 – 64.7^{o} were observed, that corresponds to the CrSi(210) and CrSi(310) planes (Fig. 3(b)).