Cr₂AlC thin film with MAX-phase structure was deposited by magnetron sputtering. Ab initio calculation of the structural was performed to obtain the relaxed lowest total energy and coordinates. Accordingly, a supercell was obtained and based on it, STEM-HAADF image was simulated with the consideration of temporal and spatial coherence of the electron beam. The result was matched with the experimental observation performed with atomic resolved STEM-HAADF images, as shown in Figure 1.

The lattice distortion in the vicinity of a growth-induced void was observed and analyzed. The distortions were observed in the vicinity of several voids, and can be as large as 23.5% of the surface layer, as shown in Fig. 2.

In order to investigate the mechanism behind the distortion, ab initio calculation was performed for simulating the surface relaxation effect, as shown in Figure 3. The ‘a’ lattice constant was controlled to shrink from 0% to 17.6%. The Cr atoms at the upper end shown in the figure are fixed and all the other atoms are allowed free to move during the relaxation calculation. As the result, the Cr-C-Cr bond was found to be expanded by as much as 49.0% in the basal plane direction while the perpendicular in-plane strain (17.6%) was applied on. Meanwhile, the Cr-Al-Cr lattices only increased by 7.2%. Although the total equilibrium energy increased from -242.3 eV to -199.5 eV by calculation, the structure remained stable therefore, the cause of the measured lattice distortion appears to be surface relaxation.
Fig. 1: Model construction, STEM-HAADF, and simulation of the HAADF pattern has been performed. The result of experiments and calculation matched as shown.

Fig. 2: A void is investigated with atomic resolved STEM-HAADF. The lattice can be distorted to the vacuum as large as 23.5% in the direction of basal plane.

Fig. 3: Ab initio calculation shows the Cr-Cr bond is much larger affected (49.0% increase) by the applied lateral compressive strain, compared to the Cr-Al-Cr bond (7.2% increase).