Pentamer with interstitial atom as the universal building block of (110), (331), (113) silicon and germanium surfaces

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Due to its technological importance, semiconductor Si and Ge have been a benchmark for studying surface physics. The major stable surfaces of Si and Ge are: (001), (111), (110), (113) and (331). These surfaces are reconstructed, i.e. topology of interatomic bonds between the surface atoms is different from that in crystal bulk. While the structure of clean (001), (111) and (113) surfaces are the most studied and their atomic and electronic structures are well established, much less was known about the structure of (110) and (331) surfaces.

In this series of works [1-9] we solved the building block structure of (110) and (331) silicon and germanium surfaces from first-principles calculations based on density functional theory and a comparison of results with available experimental scanning tunneling microscopy and spectroscopy data. The building block structure consists of the interstitial atom, which holds together five atoms of the surrounding pentamer (Fig. 1), and closely integrated rebonded area. The interstitial atom forms 6 covalent bonds with its nearest neighbors, which is unusual for atoms of group IV elements such as Si and Ge. The formation of pentamers with interstitial atoms on (110) and (331) surfaces is similar to the one previously found on (113) surfaces of Si and Ge. Thus, we demonstrated that the reconstructed (110), (113) and (331) surfaces form a family, whose members are stabilized by pentamers with interstitial atoms. All their surface structures are consistently described on a single basis.

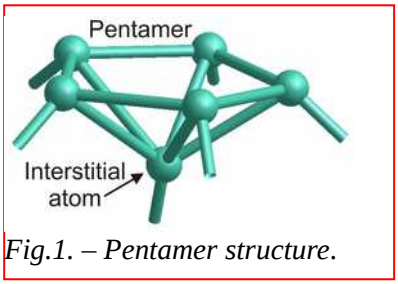

Fig.1. – Pentamer structure.

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