

# Atomic configuration of germanene, germanium counterpart of graphene

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Germanene is a germanium counterpart of graphene, i.e., a two-dimensional (2D) atomic sheet of carbon. Recently, germanene has attracted increasing attention as post-graphene materials because of its fascinating properties such as quantum spin-Hall effect [1], in addition to extremely high-carrier mobility like a graphene. This originates from the larger spin-orbit interaction in the relatively heavier atoms and the expected buckled configurations due to the bonding characters.

Germanene does not exist in nature due to the lack of parent material, like a graphite for graphene. Thus, the structure and the properties were yet to be verified experimentally. Since the pioneering works on silicene in 2012, a silicon counterpart of graphene [2-4], it has now been possible to synthesize germanene as well. In 2015, the successful fabrication of a uniform large-area germanene on an aluminum substrate was reported [5]. However, the atomic configuration of germanene had not been confirmed experimentally because of the difficulty of the structure determination for such a very thin material.

Total-reflection high-energy positron diffraction (TRHEPD) is a surface-sensitive tool owing to the positive charge of the positron (Fig. 1). The positron, an anti-particle of the electron, has the same mass and spin as the electron but the opposite sign of the electric charge. Thus, the positron beam feels a strong repulsive force from nuclei with positive point charges when approaching a material. In particular, the total reflection takes place at grazing incidence, where the penetration depth is limited to the thickness of one atomic layer. Therefore, the TRHEPD technique is suitable for the structure determination of 2D atomic sheets such as germanene.

According to the previous theoretical works, two Ge atoms (labelled 2 and 7 in the right part of Fig. 2) in the unit cell were shifted upwards, as a symmetric structure [5]. However, the TRHEPD experiments demonstrated that the diffraction pattern observed is asymmetric, contrary to the theoretical expectation. The intensity analysis based on dynamical diffraction theory revealed that only one Ge atom (labelled 7 in the left part of Fig. 2) is shifted upwards [6]. As a result, we found that the germanene has an asymmetric structure, unlike a symmetric one expected in the previous studies. The newly proposed structure is expected to reveal the novel physical properties of germanene

## References

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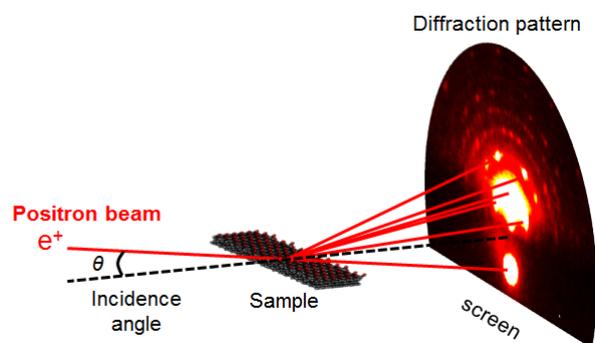


Fig.1 Experimental setup for TRHEPD method. The positron beam with an energy of 10 keV is reflected at a sample surface, and then the diffraction pattern is observed on a screen.

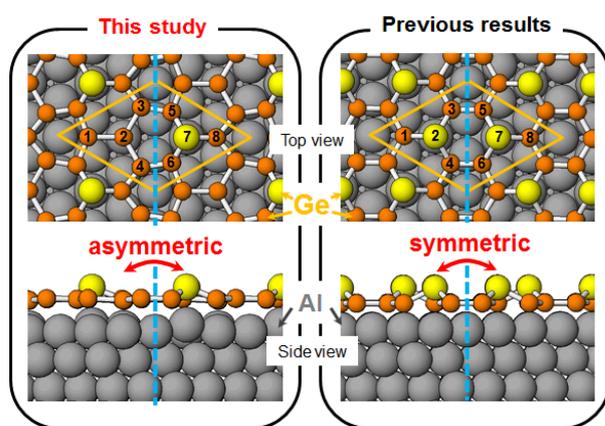


Fig.2 Atomic configurations of germanene on an aluminium substrate determined in this study (left) and expected in the previous studies (right). Yellow and orange circles denote Ge atoms and gray ones are Al atoms. The upwardly shifted Ge atoms are highlighted as enlarged circles for guide to eyes.