MS111.O01

Structure determination of two-dimensional atomic sheet of silicene using TRHEPD

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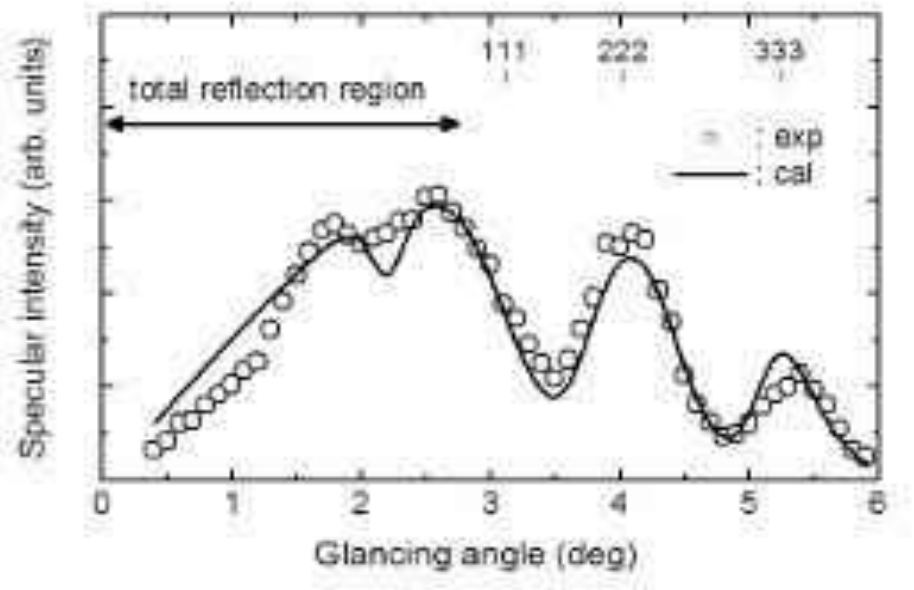
This study reports determination of the atomic coordinates of a two-dimensional atomic sheet, silicene, by using total reflection high-energy positron diffraction (TRHEPD) [1]. TRHEPD method, formerly called as RHEPD, is a surface-sensitive tool owing to the total reflection of positrons. Since the sign of the potential energy for positrons in crystals is positive, opposite to that for the electrons, the positron beam at a grazing incidence are totally reflected at a crystal surface. The penetration depth of the positron beam in the total reflection region is estimated to be approximately a few Å, which corresponds to the thickness of 1-2 atomic layers. Thus, the positron beam selectively sees the topmost surface layer and hence the TRHEPD method is very useful for structure determinations of crystal surface and two-dimensional atomic sheet on the substrate. Silicene is a two-dimensional atomic sheet of silicon. Since the silicene has an intriguing property such as a Dirac cone like a graphene, it attracts increasing attention as a candidate for future devices. Recently, the synthesis of silicene on a Ag(111) surface was successfully performed [2]. Although the atomic coordinates of the silicene in this system was theoretically calculated, they were not confirmed experimentally. It is very important to experimentally determine the magnitude of the buckling in silicene and the spacing between the bottom of the silicene and the substrate because the dispersion of the Dirac cone is closely related to these structure parameters. We thus investigated the atomic positions of the silicene on the Ag(111) surface using the TRHEPD [3]. From the rocking curve analysis based on the dynamical diffraction theory of positrons (see figure), the existence of the buckling (0.83 Å) in silicene was verified experimentally. Moreover, the spacing between the silicene and the substrate was determined as 2.17 Å. The structural difference with the graphene will be also discussed.

[1] *Y. Fukaya, M. Maekawa, A. Kawasuso, et al., to be published in Appl. Phys. Express, 2014,* ***[2]*** *P. Vogt, P. De Padova, C. Quaresima, et al., Phys. Rev. Lett., 2012, 108, 155501,* ***[3]*** *Y. Fukaya, I. Mochizuki, M. Maekawa, et al.o, Phys. Rev. B, 2013, 88, 205413*



Keywords: silicene, positron diffraction, total reflection