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Identifying Antisite and Vacancy Defects in n-doped Bi_2Se_3 Topological Insulators from Scanning Tunneling Microscopy and First Principles Calculations JEONG HEUM JEON, Department of Physics, Korea University, Seoul, 136-713, Republic of Korea, JOON-SUH PARK, Department of Physics, Yonsei University, Seoul 120-749, Republic of Korea, HOWON KIM, WON JUN JANG, Department of Physics, Korea University, Seoul, 136-713, Republic of Korea, JINHEE HAN, HYUNGJUN LEE, HYUNG-JOON CHOI, Department of Physics, Yonsei University, Seoul 120-749, Republic of Korea, SE-JONG KAHNG, Department of Physics, Korea University, Seoul, 136-713, Republic of Korea — Intrinsic defects are the major sources of n-type doping character in Bi_2Se_3 topological insulators, but their structural nature remains unsettled; Theoretical calculations predicted that Se_{Bi} antisite was the most preferred under Se-rich, i.e. molecular beam epitaxy conditions, but there has been no report on its experimental observation. Here, we present our energy-dependent atomic resolution scanning tunneling microscopy (STM) images for intrinsic defects obtained from Bi_2Se_3 thin films grown under Se-rich conditions. We observed two types of defects, and identified them as Se_{Bi} antisite and Bi vacancy located at Bi layer right below surface Se layer, by comparing experimental STM images with the simulated ones obtained from first principles calculations. Our study shows that, in agreement with previous predictions, not Se-vacancy at surface but Se_{Bi} antisite is the origin of n-type doping in our Bi_2Se_3.

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