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Structural study of topological insulator $\mathbf{Bi_2(Se_{3-x}Te_x)}$

KEESEONG PARK, University of Virginia, Charlottesville, Virginia 22904, USA., DESPINA LOUCA, University of Virginia, Charlottesville, Virginia 22904, USA, ANNA LLOBET, Lujan Neutron Scattering Center, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA — With neutron diffraction, we systematically investigated the local and average structures of topological insulator $Bi_2(Se_{3-x}Te_x)$ (x=0, 1, 1.5, 2, and 3) from 5 to 500 K. The average crystal structure of Bi_2Se_3 is rhombohedral R-3m symmetry with 2 unique chalcogen sites. This gives rise to 2 types of Bi-(Se/Te) bonds in quintuple layer composed of Se1-Bi-Se2 –Bi-Se1 layers, covalent Se1-Bi bond with the bonding length of 2.85 Å and ionic Se2-Bi bond with the bonding length of 3.07 Å at 5 K. The Se1-Se1 bonds between quintuple layers are governed by Van der Walls of the length of 3.47 Å at 5 K. With increasing temperature, it is observed that the quintuple layer unit contracts from the anti-parallel motion of the Bi-$(Se1)_3$ tetrahedra toward the Se2-center layer. Also such a contraction implies the Van der Waals bonding between quintuple layers weakens with temperature. A similar temperature dependence of atomic structure is observed on Bi_2Se_3.

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