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Emergent Topological States at Domain Walls in Bismuth[1] JINWOONG KIM, NICHOLAS KIOUSSIS, Department of Physics and Astronomy, California State University, Northridge — The discovery of topological insulators has brought new perceptions in materials science which allows the understanding of material properties as an inevitable result of symmetry and its breaking. Polyacetylene is one example of topological insulators classified by structural symmetry that exhibits zero modes at a domain wall separating two opposite dimerized phases. The sign reversal of the topological mass across a domain wall is not restricted to 1D systems and is ubiquitous in a wide range of 3D materials. Employing both ab initio and model Hamiltonian calculations we have studied the topological properties of structural domain walls in bismuth, which is the 3D analogue of the domain walls in 1D polyacetylene. The model Hamiltonian can be represented to lowest order by two Pauli matrices yielding a mass gap that closes upon dimerization sign reversal. The calculations demonstrate that zero mode states emerge at the domain wall which exhibit quasi-one dimensional linear dispersions. Our results imply that conducting channels may emerge at structural domain walls such as grain boundaries as a consequence of topological protection, whose properties are determined by global rather than local symmetry.

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