Understanding High-Pressure Formation of Topologically Non-trivial Intermetallic Compounds via In-Situ X-ray Diffraction

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The investigation of topologically non-trivial surface states is at the forefront of condensed matter physics and material science. Of particular interest is the concurrence of non-trivial topology with superconductivity which has sparked both fundamental questions about the intersection of these phenomena and revealed potential applications in quantum computing. Although the extensive exploration of temperature–composition phase spaces has enabled experimental realization of topologically non-trivial compounds, very few superconduct. This paucity of topologically non-trivial superconductors creates an impetus for alternate synthetic routes to discover new topologically non-trivial superconductors. A key criterion for accessing non-trivial topology is the combination of a large degree of spin–orbit coupling and mobile electrons in the correct symmetry. To realize new topologically non-trivial superconductor candidates, we chose to combine lead, the largest, non-radioactive, main-group element, as a source of spin-orbit coupling with transition metals as a source of mobile electrons. As lead reacts with late-transition metals to form superconducting intermetallic compounds and many transition-metal–lead binary compounds have suitable symmetry for non-trivial topology, we chose to target binary compounds that combine late-transition metals with lead as promising candidates for topologically non-trivial superconductivity. Among these binary systems, a few, such as, Ni–Pb, had no thermodynamically stable compounds reported despite thorough investigation of their binary temperature–composition phase space. By combining high-pressure, high-temperature synthesis with in-situ and ex-situ X-ray diffraction techniques, we synthesized and crystallographically characterized the first intermetallic compound in the Ni–Pb system, Ni_3Pb_2. The pseudo-hexagonal symmetry within the modulated Ni_3Pb_2 structure and the Dirac cones predicted at the Fermi energy of the band structure suggest Ni_3Pb_2 may exhibit non-trivial topology. Moreover, Ni_3Pb_2 is recoverable to ambient conditions enabling further investigation of its electronic properties. Here, we present the high-pressure synthesis of Ni_3Pb_2, our insight into its formation, and our progress investigating its properties.