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Topological nodal line semimetal: Zirconium di-arsenide

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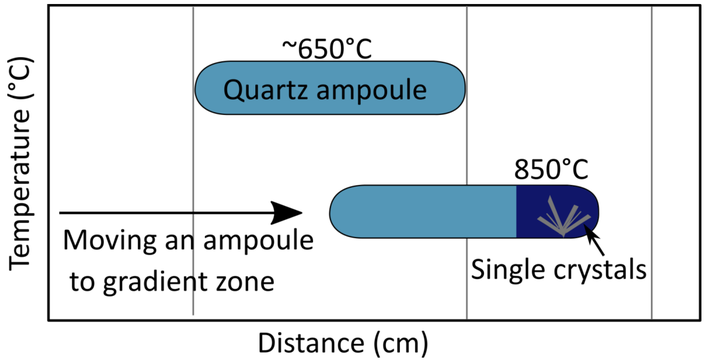
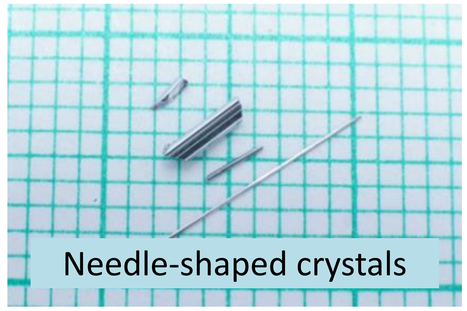
Motivation

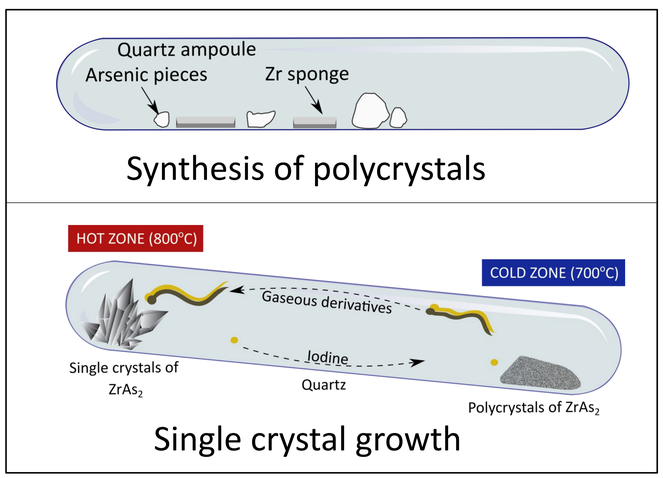
- The conduction and valence bands intersect along a one-dimensional path within the three-dimensional Brillouin zone. Furthermore, any external influence or perturbation applied to the system maintains a specific symmetry group. This material possess the non-symmorphic symmetry along with the inversion and time reversal symmetry.
- Nodal lines give rise to extremely large magnetoresistance, SdH oscailltions and symmetry enforced band crossings
- Studying the single crystals by angle-resolved photoemission spectroscopy (ARPES) with DFT support helps us understand better how various symmetries are structured and impact the topological properties.

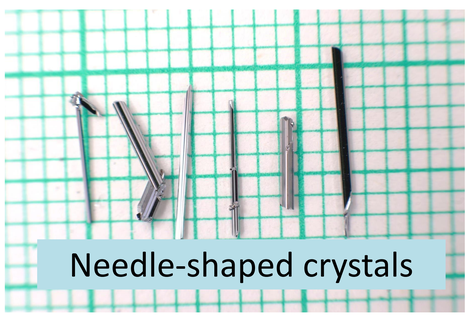
One-step process



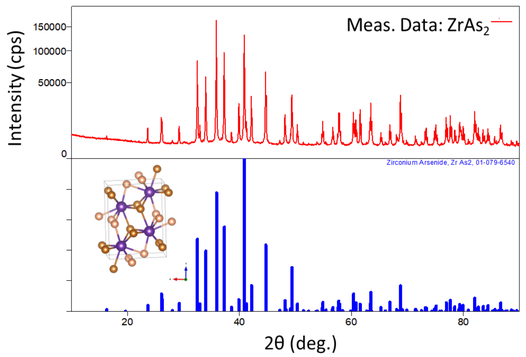


Two-step process

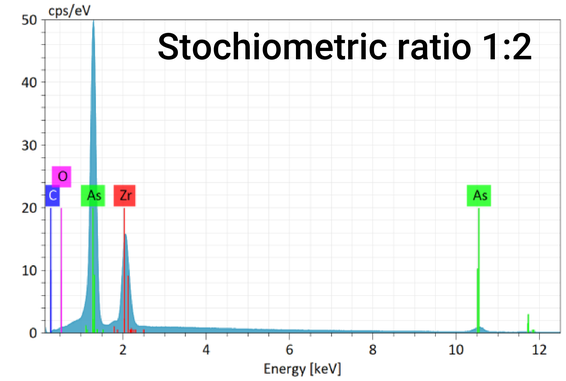




Lattice parameters
a = 6.801 Å, b = 9.033 Å, c = 3.688 Å

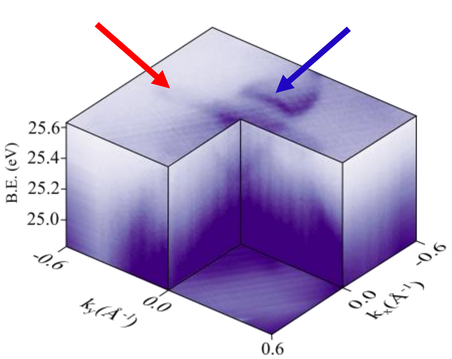


X-ray diffraction (inset) crystal structure



EDX spectrum

DFT calculations before and after inclusion of SOC



3D ARPES with Fermi pockets shown by arrows

Summary

1. CVT method: Needle shaped-crystals (in both the processes)
2. Orthorhombic crystal structure (Pnma 62), centrosymmetric, TRS protected
3. Stochiometry 1:2
4. Accidental degereacies lifted with SOC
5. 3D ARPES plot shows electron and hole pockets

References

- J. Alloys Compd. 505, 17 (2010)
- Phys. Rev. B 104, 125135 (2021)
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