TlCu5Se3– Unusual Wave-like Thermal Transport

Prelims: *Current events of national and international importance | Science & Technology*

Why in News?

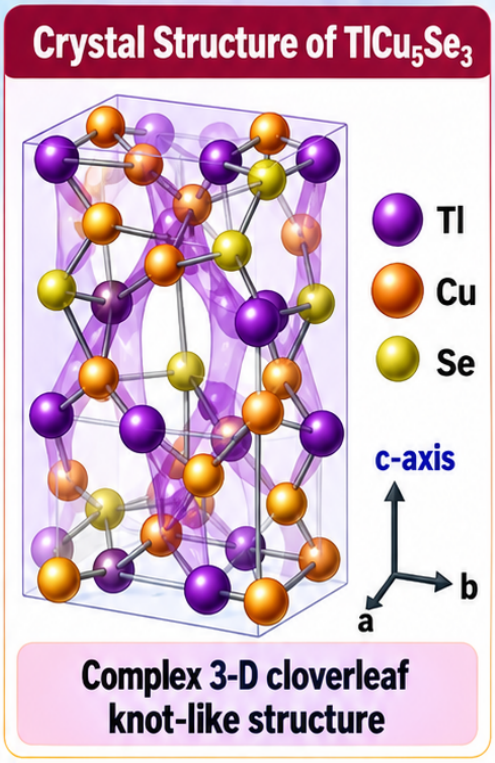
*A team from **JNCASR, Bengaluru**, in collaboration with other researchers, has identified an unusual **wave-like thermal transport regime** in the copper chalcogenide **thallium copper selenide.***

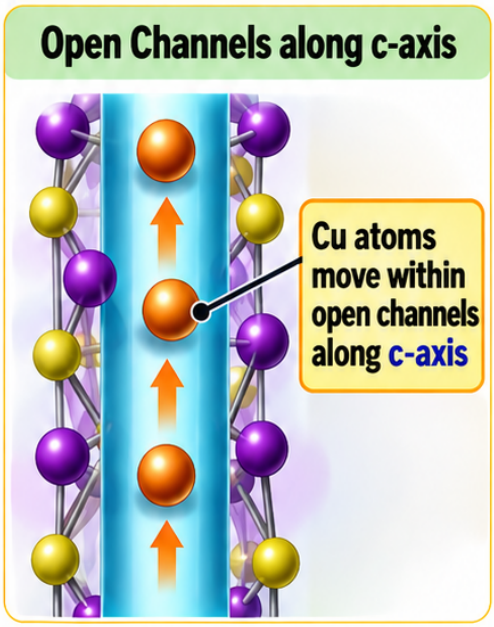
- **Material studied –** Thallium copper selenide (TlCu5Se3), a copper chalcogenide.

SHANKAR IAS PARLIAMENT

Key Features of $TlCu_5Se_3$

Feature	$TlCu_5Se_3$
Material class	Copper chalcogenide
Crystal structure	Tetragonal
Framework	Complex 3-D cloverleaf knot-like structure
Channels	Open channels along c-axis
Mobile species	Cu atoms
Cu behaviour	Confined/localized dynamic disorder
Lattice thermal conductivity	Ultralow
Thermoelectric zT	1.7





- **Conducted at –** JNCASR, Bengaluru, an autonomous institution under the Department of Science & Technology.
- **Key discovery –** An **unusual wave-like thermal transport regime,** attributed to confined copper atom dynamics within a complex crystal framework.
- **Result –** The material exhibits intrinsically ultralow lattice thermal conductivity and favorable electronic transport, leading to high thermoelectric performance with a zT of

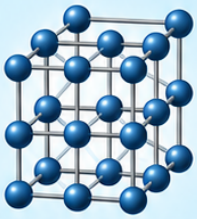
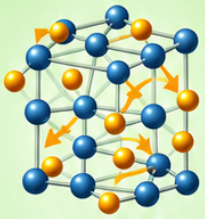
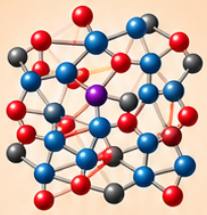
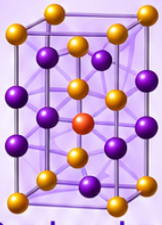
approximately 1.7, which is notable among pristine ternary chalcogenides.

- **Potential applications –** It include thermoelectric energy conversion in
  - Power plants,
  - Cement and steel industries,
  - Automobiles, and data centers,
  - Battery heat management and
  - Thermal barrier coatings.

Thermoelectric Energy Conversion
• **Thermoelectric materials** enable the direct conversion of temperature gradients **into electrical energy**. • **Key Parameter** – **The thermoelectric figure of merit (zT)** is a critical parameter; a higher zT value typically signifies improved thermoelectric conversion efficiency.

SHANKAR IAS PARLIAMENT

Comparison of Thermal and Structural Properties: Conventional, Superionic, Glassy Materials and $TlCu_5Se_3$

Parameter	Conventional Crystalline Materials	Superionic Materials	Glassy / Highly Disordered Materials	$TlCu_5Se_3$
	 Ordered crystal	 Crystal with highly mobile ions	 Highly disordered structure	 Complex, ordered tetragonal crystal
Structure	Ordered crystal	Crystal with highly mobile ions	Highly disordered	Complex, ordered tetragonal crystal
Ion movement	Relatively restricted	Long-range / liquid-like ion migration	Random atomic disorder	Confined/localized Cu dynamics
Heat carriers	Mainly particle-like phonons	Phonons affected by mobile ions	Conventional phonon propagation strongly suppressed	Particle-like + wave-like transport
Phonon behaviour	Well-defined propagation	Strongly affected by ion mobility	MFP approaches interatomic distance	Phonons can tunnel between localized vibrational states
Anharmonicity	Relatively lower	Can be significant	Strong	Exceptionally strong
Thermal conductivity	Generally higher	Low	Very low	Ultralow lattice thermal conductivity
Structural stability	Generally stable	Excessive ion migration may cause instability	Disorder dominates	Confined Cu motion helps retain stability
Nature of thermal transport	Mainly particle-like	Mainly phonon-based with ionic disorder	Suppressed phonon propagation	Predominantly wave-like coherence
Thermoelectric potential	Depends on material	Can be high but stability can be an issue	Potentially high	High; $zT = 1.7$

Anharmonicity *refers to the deviation of atomic vibrations from ideal harmonic or parabolic behavior.*

Reference

DST | Unusual Wave-Like Heat Transport in Crystalline Solid