Discovery of Unusual Structural and Electronic Properties in Monolayer and Multilayer Si_2Te_3.

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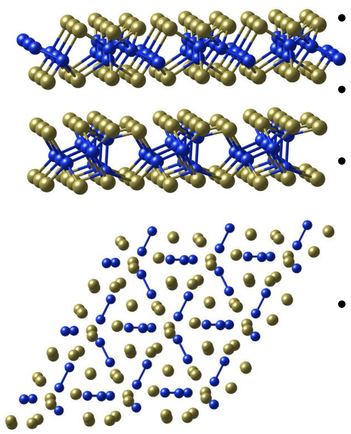
Introduction



- Layered 2-dimensional crystal structure
- Tellurium forms a hexagonal close packed lattice.
- Silicon dimers occupy interstitial sites in alternating layers (Keuleyan et al. 2015).
- The silicon dimers are able to switch between four possible orientations at room temperature.

Method

Density Functional Theory

- Density Functional Theory allows total energy calculations to deal directly with the density of electrons instead of individual particles.

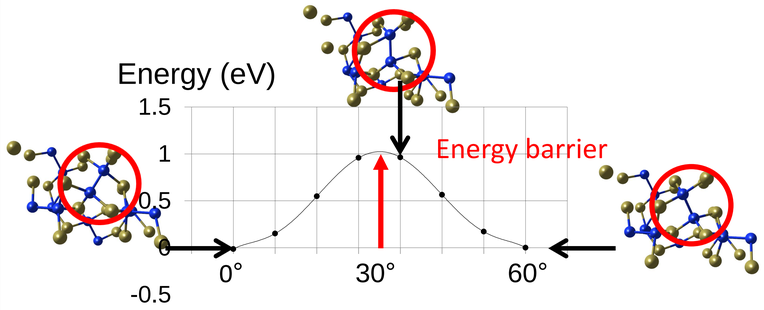
$$\hat{H}\Psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_N) = E\Psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_N)$$

- Using electron density instead of considering every electron-electron interaction makes the simulation computationally efficient.

$$\Psi(\vec{x}_1, \vec{x}_2, ..., \vec{x}_N) \rightarrow \rho(\vec{r})$$

$$\rho(\vec{r}) \rightarrow E$$

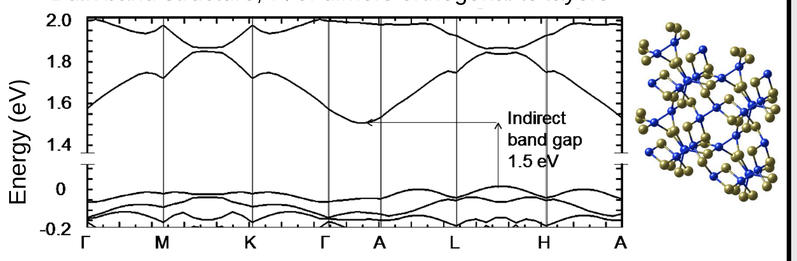
Results



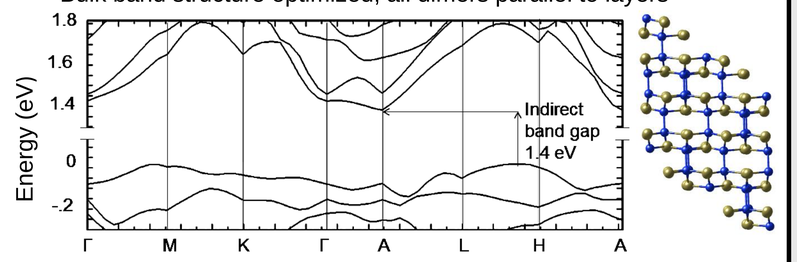
- We calculated the energy barrier of one of these changes in silicon dimer orientation to be about one eV.
- The energy barrier is small enough so that the dimers can change orientation at room temperature.

Electron Band Structure

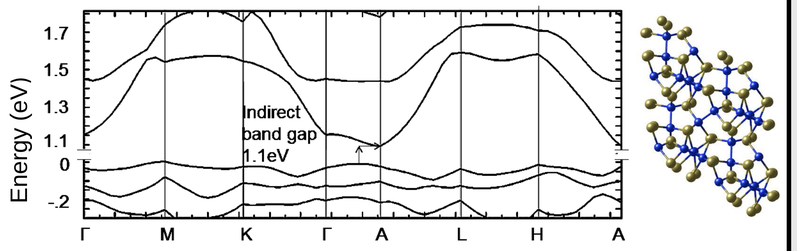
Bulk band structure, ¼ of dimers orthogonal to layers



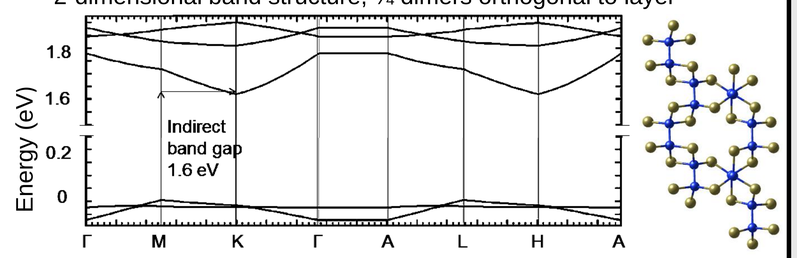
Bulk band structure optimized, all dimers parallel to layers



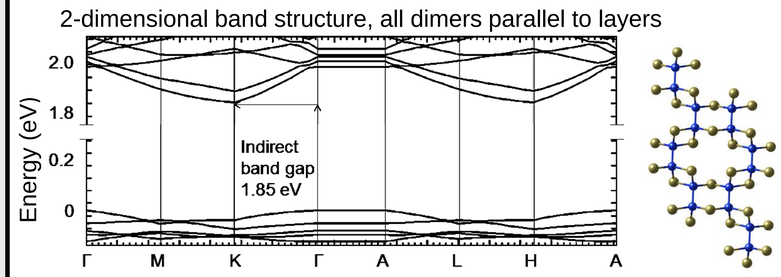
Bulk band structure with dimers at random orientation



2-dimensional band structure, ¼ dimers orthogonal to layer



2-dimensional band structure, all dimers parallel to layers



- The different band structure diagrams displayed show that differences in the silicon dimer configuration in silicon telluride largely affect the band gap and shape of the band structure. This means that the material has highly temperature dependent electronic properties.

Conclusion

- Si_2Te_3 is a 2-dimensional layered crystal structure with a variable band gap due to silicon dimers that can change orientation.
- Change in silicon dimer orientation is accompanied by a five percent change in lattice constant. Because of this, strain could be used to influence the orientation of the silicon dimers.
- The variability of the electron band structure of this material could potentially make it useful in optical and thermal sensing applications.

References

(1) Keuleyan, S.; Wang, M.; Chung, F. R.; Commons, J.; Koski, K. J. Nano Lett. 2015, 15 2285-2290.

Acknowledgements

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