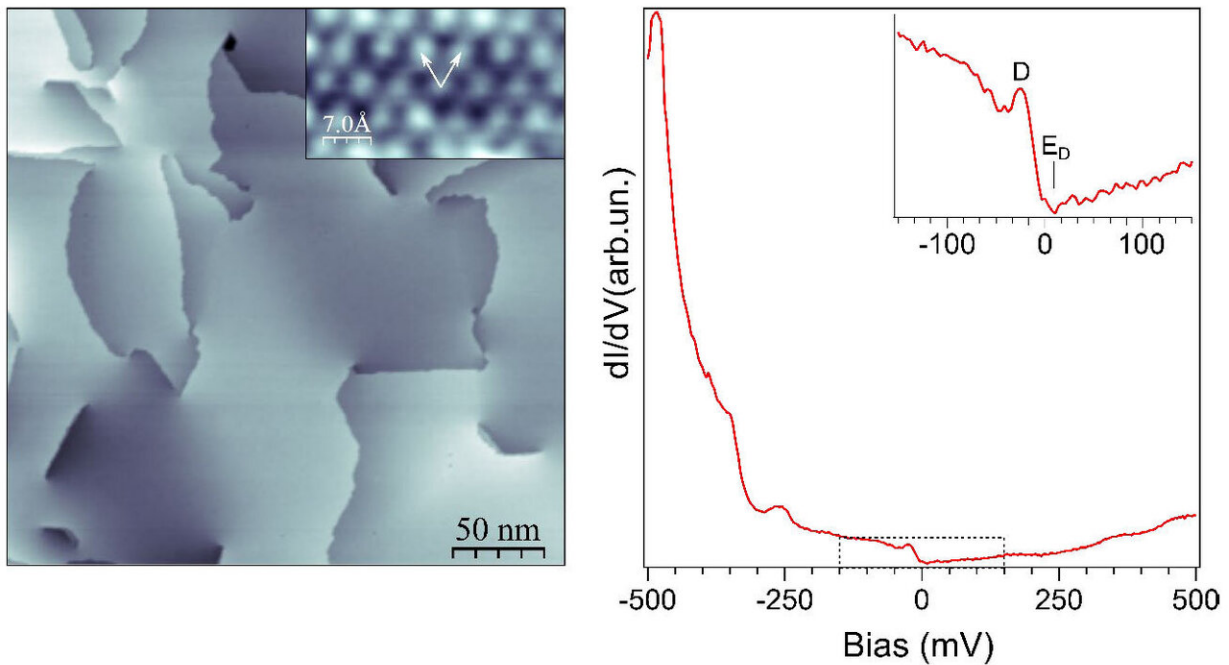


Unexpectedly fast conduction electrons in Na₃Bi

August 17 2020, by Iolanda Di Bernardo



Left: STM image showing topography of Na₃Bi sample. Right: Density of states showing a minimum at the Dirac point E_D . Credit: FLEET

An Australian-led study uses a scanning-tunneling microscope "trick" to map electronic structure in Na₃Bi, seeking an answer to that material's extremely high electron mobility.

In studying the topological Dirac semimetal, the team found that

exchange and correlation effects are crucial to electron speed, and therefore mobility, and thus to the use of this exciting class of materials in future ultra-low energy electronics.

To date, little has been known about the band dispersion of Na_3Bi in the conduction band (above the Fermi level), though there have been tantalizing hints that the actual velocity of the electrons is much larger than theoretical predictions.

"We grew thin films of Na_3Bi and investigated their band structure via quasiparticle interference," says lead author Dr. Iolanda di Bernardo.

"Our calculations revealed that to understand the extremely high experimental velocities of the charge carriers, particularly in the conduction band, exchange and correlation effects are crucial."

Clever tricks and surprises

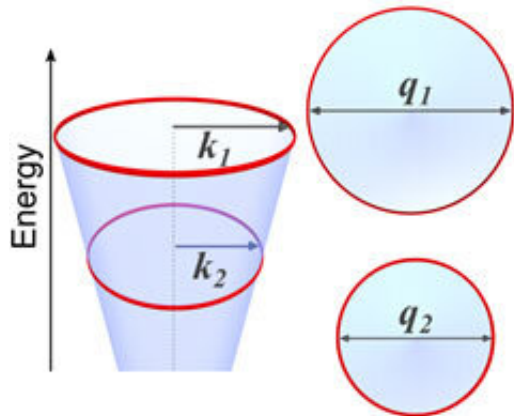
Topological Dirac semimetals can be considered as the 3-D counterparts of graphene: around the Fermi level (where the conduction electrons "usually" sit) they exhibit the same linear band dispersion that graphene does, which means that their electrons are virtually massless.

This, naturally, translates into extremely high conductivity, and in this case, occurs in all three directions in space.

This linear band dispersion was predicted for Na_3Bi , but a proper mapping of the [conduction band](#) for this material was still missing.

Measuring the band structure of materials above the Fermi level is, in fact, not a trivial task—mainly because electrons are not typically occupying these states.

One of the few ways this can be accomplished is by using a trick based on scanning tunneling spectroscopy:



The circular shape of constant-energy contours (mapped in reciprocal space) correspond to conic sections of a Dirac-cone. Credit: FLEET

"We acquire 'mappings' of the quantum tunneling current between the tip and the sample at different biases," explains Iolanda.

The derivatives of these mappings show very typical patterns, originating from the scattering of the electrons with the disorder in the sample.

This scattering process mixes electrons that are on the same constant-energy contours in reciprocal space, which is made visible by taking a Fourier transform of the mappings.

"In our case, this yielded circles corresponding to cuts along a Dirac-cone like dispersion." (see figure).

This analysis technique allowed the team to reconstruct the (linear) band dispersion in the material and extract the charge carriers' velocities, both

in the valence and the conduction bands.

But when these measured band dispersions were compared with theoretical predictions, there was a problem: the measured velocities for the lowest-lying conduction and valence bands were significantly higher than theoretical predictions.

However, the team found one way to significantly improve agreement between measurement and theory:

"We used increasingly complicated models to describe our system, and discovered that as we improved the treatment of the exchange and correlation potential in the model (going from PBE to GW methods), we could get closer to the experimental values—even though we still observed some discrepancies," explains Iolanda.

While the origin of these unexpectedly [strong interactions](#) is still unclear, the new study demonstrates that exchange-correlation effects are likely at the base of the high velocity of electrons in Na₃Bi.

Understanding the ultra-high mobilities of carriers in topological Dirac semimetals is a step toward the successful implementation of these materials in devices for low-energy electronics.

The study, titled "Importance of interactions for the band structure of the topological Dirac semimetal Na₃Bi," was published in July 2020 in *Physical Review B*.

More information: I. Di Bernardo et al. Importance of interactions for the band structure of the topological Dirac semimetal Na₃Bi, *Physical Review B* (2020). [DOI: 10.1103/PhysRevB.102.045124](https://doi.org/10.1103/PhysRevB.102.045124)

Provided by FLEET

Citation: Unexpectedly fast conduction electrons in Na₃Bi (2020, August 17) retrieved 25 April 2024 from <https://phys.org/news/2020-08-unexpectedly-fast-electrons-na3bi.html>

This document is subject to copyright. Apart from any fair dealing for the purpose of private study or research, no part may be reproduced without the written permission. The content is provided for information purposes only.