

placed. During a typical extraction, water is pumped to the required high pressure through supply valves, a pre-heating coil, the sample cell, and an analyte valve into a collection vial. The filters, at various positions downstream of the sample cell, prevent contamination of analytical instruments by particles of the sample solid matrix.

Relative to prior methods and apparatuses used to extract organic compounds, the present apparatus and the

method of its operation offer several advantages:

- The solvent (water) is environmentally benign;
- The relative permittivity of the solvent can be adjusted to the values needed to selectively extract, with high efficiency, organic compounds that have different physical and chemical properties;
- The basic principle of operation is simple;
- The apparatus can be highly automated;

- Whereas Soxhlet and hydrolysis extractions often take many hours, an extraction by use of this apparatus takes only minutes.

This work was done by Xenia Amashukeli, Frank Grunthaler, Steven Patrick, James Kirby, Donald Bickler, Peter Willis, Christine Pelletier, and Charles Bryson of Caltech for NASA's Jet Propulsion Laboratory. Further information is contained in a TSP (see page 1). NPO-44144

A Model for Predicting Thermoelectric Properties of Bi_2Te_3

A compromise between accuracy and computational efficiency is made.

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A parameterized orthogonal tight-binding mathematical model of the quantum electronic structure of the bismuth telluride molecule has been devised for use in conjunction with a semi-classical transport model in predicting the thermoelectric properties of doped bismuth telluride. This model is expected to be useful in designing and analyzing Bi_2Te_3 thermoelectric devices, including ones that contain such nanostructures as quantum wells and wires. In addition, the understanding gained in the use of this model can be expected to lead to the development of better models that could be useful for developing other thermoelectric materials and devices having enhanced thermoelectric

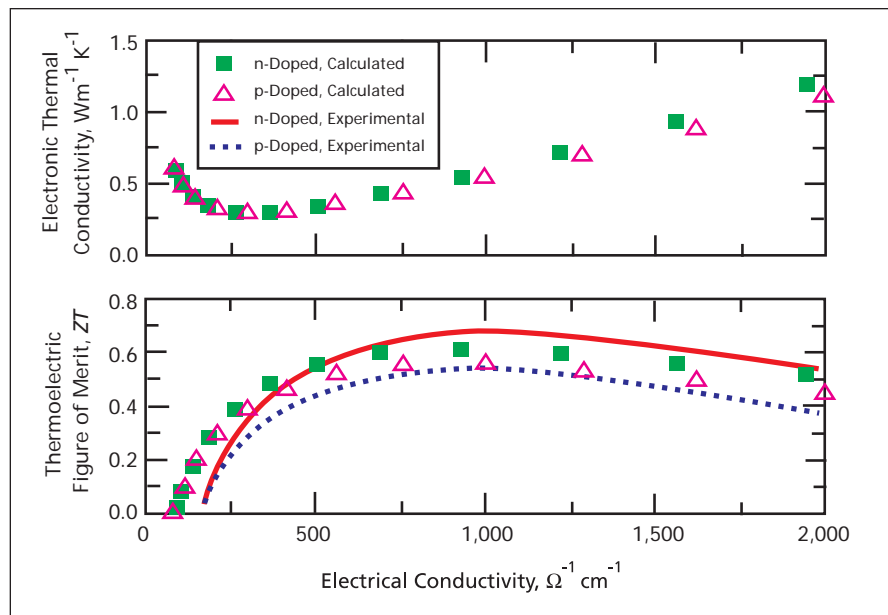
properties.

Bi_2Te_3 is one of the best bulk thermoelectric materials and is widely used in commercial thermoelectric devices. Most prior theoretical studies of the thermoelectric properties of Bi_2Te_3 have involved either continuum models or *ab-initio* models. Continuum models are computationally very efficient, but do not account for atomic-level effects. *Ab-initio* models are atomistic by definition, but do not scale well in that computation times increase excessively with increasing numbers of atoms. The present tight-binding model bridges the gap between the well-scalable but non-atomistic continuum models and the atomistic but poorly scalable *ab-initio* models:

The present tight-binding model is atomistic, yet also computationally efficient because of the reduced (relative to an *ab-initio* model) number of basis orbitals and flexible parameterization of the Hamiltonian.

The present tight-binding model includes atomistic descriptions of the Hamiltonian with $sp^3d^5s^*$ basis orbitals, nearest-neighbor interactions, and spin-orbit coupling. For the purposes of the model, within each primitive cell of Bi_2Te_3 , two of the Te atoms are denoted Te^I and one is denoted Te^{II} . The difference between Te^I and Te^{II} is that the nearest neighbors of Te^I are three Te atoms and three Bi atoms, while those of Te^{II} are six Bi atoms. To capture the difference, separate tight-binding parameters are assigned to Te^I and Te^{II} .

Altogether, the tight-binding model incorporates 71 independent parameters, which are determined by fitting the computed band structure to a first-principles band structure obtained by use of a submodel based on a screened-exchange local-density approximation. The first-principles band structure predicts the energy gap, the degeneracy of the edges of the conduction and valence bands, and the effective masses of these two bands, in good agreement with experimental results. In the fitting process, a higher priority is given to the highest valence and the lowest conduction bands than to the rest of the band structure, inasmuch as these two bands are mainly responsible for the thermoelectric properties of lightly doped Bi_2Te_3 . Moreover, the locations, energies, and effective masses of the two band edges are emphasized, as they largely determine the accuracy of the



Calculated and Experimental Values of the thermoelectric figure of merit and the electronic thermal conductivity of Bi_2Te_3 were found in fairly close agreement across a broad range of electrical conductivity.

thermoelectric properties predicted by use of this model.

The semiclassical transport model with which this tight-binding model is coupled is a solution of Boltzmann's transport equation in the constant-relax-

ation-time approximation. The combination of models has been found to yield calculated values of thermoelectric properties within a few percent of experimentally determined values (for example, see figure).

This work was done by Seungwon Lee and Paul Von Allmen of Caltech for NASA's Jet Propulsion Laboratory. For more information, contact iaoffice@jpl.nasa.gov. NPO-43777

Integrated Miniature Arrays of Optical Biomolecule Detectors

Many biochemical species could be detected simultaneously.

NASA's Jet Propulsion Laboratory, Pasadena, California

Integrated miniature planar arrays of optical sensors for detecting specific biochemicals in extremely small quantities have been proposed. An array of this type would have an area of about 1 cm². Each element of the array would include an optical microresonator that would have a high value of the resonance quality factor ($Q \approx 10^7$). The surface of each microresonator would be derivatized to make it bind molecules of a species of interest, and such binding would introduce a measurable change in the optical properties of the microresonator. Because each

microresonator could be derivatized for detection of a specific biochemical different from those of the other microresonators, it would be possible to detect multiple specific biochemicals by simultaneous or sequential interrogation of all the elements in the array. Moreover, the derivatization would make it unnecessary to prepare samples by chemical tagging.

Such interrogation would be effected by means of a grid of row and column polymer-based optical waveguides that would be integral parts of a chip on which the array would be fabricated. The row

and column polymer-based optical waveguides would intersect at the elements of the array (see figure). At each intersection, the row and column waveguides would be optically coupled to one of the microresonators. The polymer-based waveguides would be connected via optical fibers to external light sources and photodetectors. One set of waveguides and fibers (e.g., the row waveguides and fibers) would couple light from the sources to the resonators; the other set of waveguides and fibers (e.g., the column waveguides and fibers) would couple light from the microresonators to the photodetectors. Each microresonator could be addressed individually by row and column for measurement of its optical transmission. Optionally, the chip could be fabricated so that each microresonator would lie inside a microwell, into which a microscopic liquid sample could be dispensed.

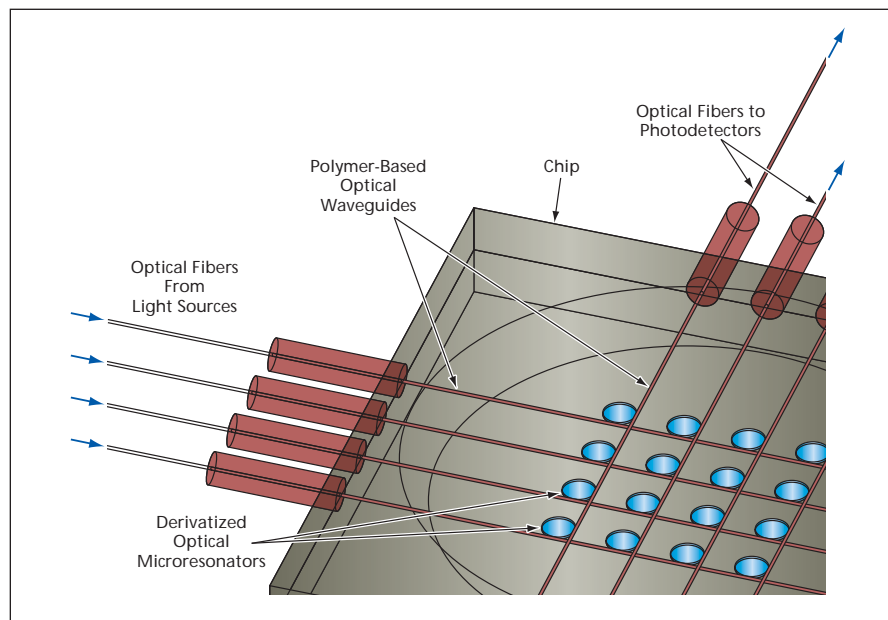
This work was done by Vladimir Ilchenko, Lute Maleki, Ying Lin, and Thanh Le of Caltech for NASA's Jet Propulsion Laboratory.

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Refer to NPO-43164, volume and number of this NASA Tech Briefs issue, and the page number.



Derivatized Optical Microresonators in an array would address optically via row and column optical waveguides.