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Electron and phonon thermal conductivity in high entropy carbides with variable carbon content

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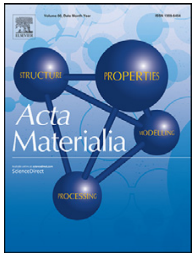

Full length article

Electron and phonon thermal conductivity in high entropy carbides with variable carbon content

Christina M. Rost[a,b], Trent Borman[c], Mohammad Delower Hossain[c], Mina Lim[d], Kathleen F. Quiambao-Tomko[e], John A. Tomko[e], Donald W. Brenner[d], Jon-Paul Maria[c], Patrick E. Hopkins[a,e,f,*]

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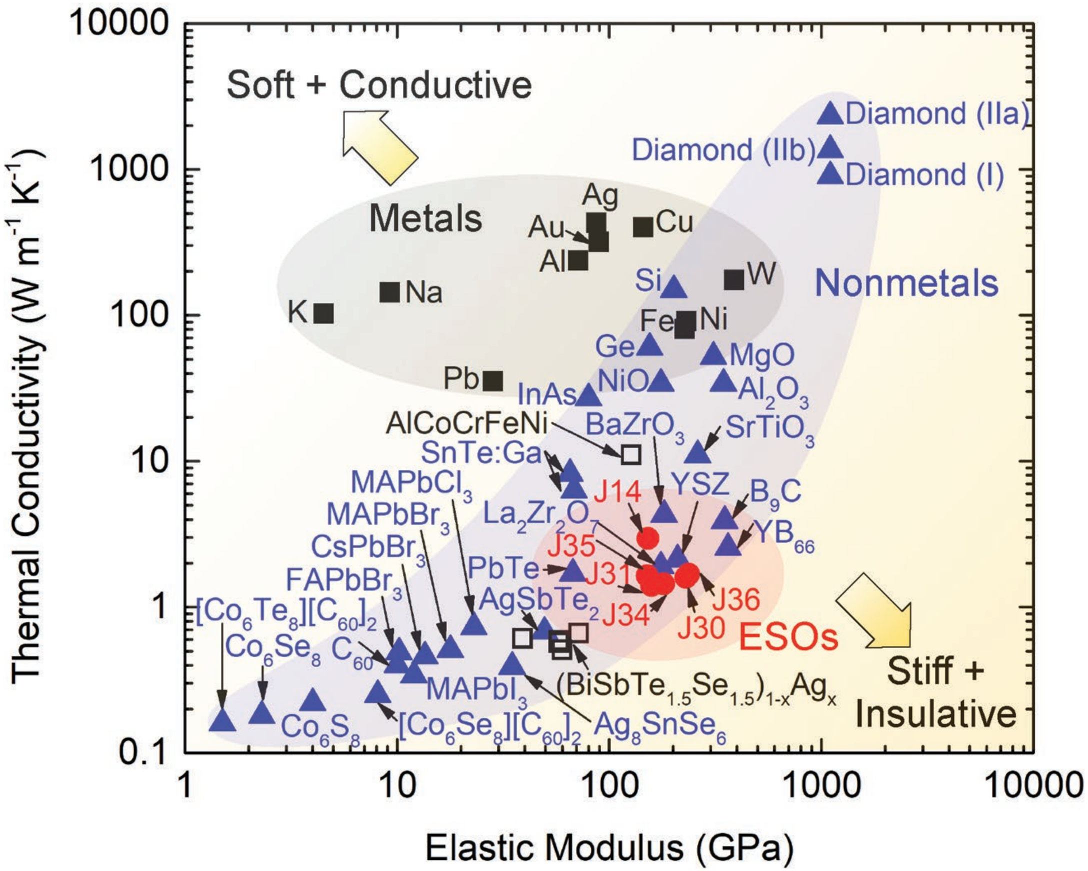
[b] *Department of Physics and Astronomy, James Madison University, Harrisonburg, VA 22807, USA*
[c] *Department of Materials Science and Engineering, The Pennsylvania State University, University Park, PA 16802, USA*
[d] *Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC 27695, USA*
[e] *Department of Materials Science and Engineering, University of Virginia, Charlottesville, VA 22904, USA*
[f] *Department of Physics, University of Virginia, Charlottesville, VA 22904, USA*

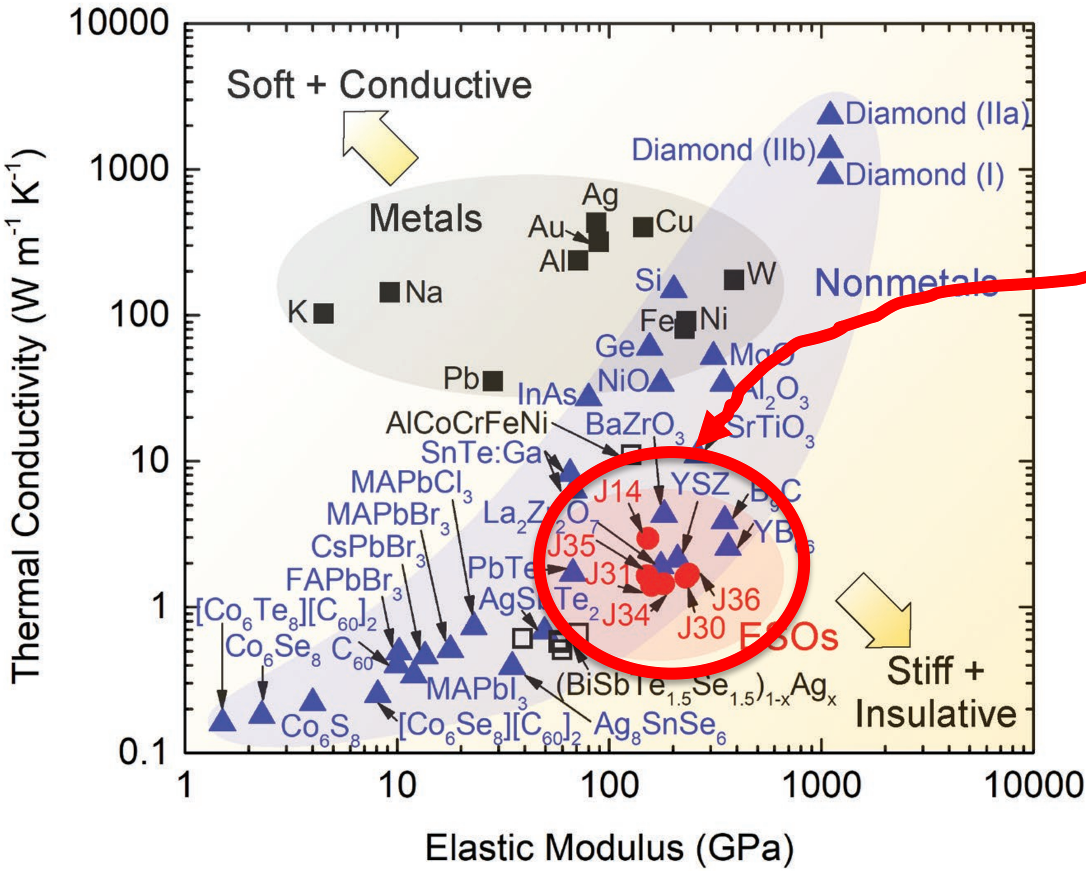
Thermal conductivity – the "mechanical" perspective

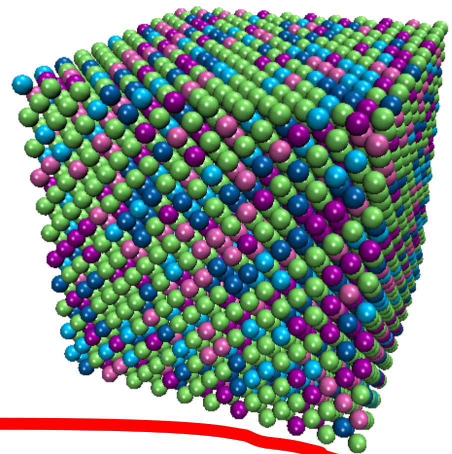


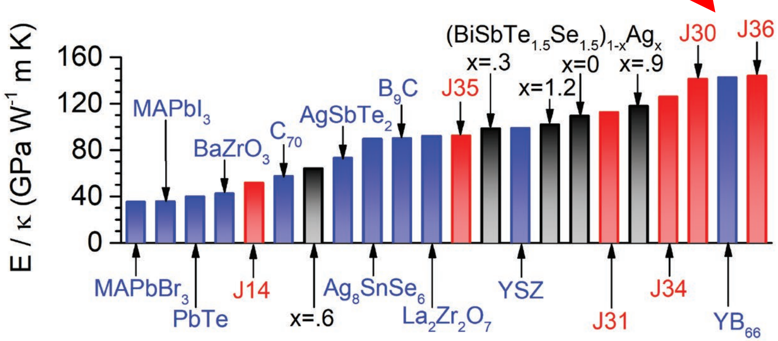
$$\kappa \propto \frac{E}{M_{\mathrm{avg}}}$$

Adv. Mat. **30**, 1805004 (2018)

Thermal conductivity of high entropy oxides

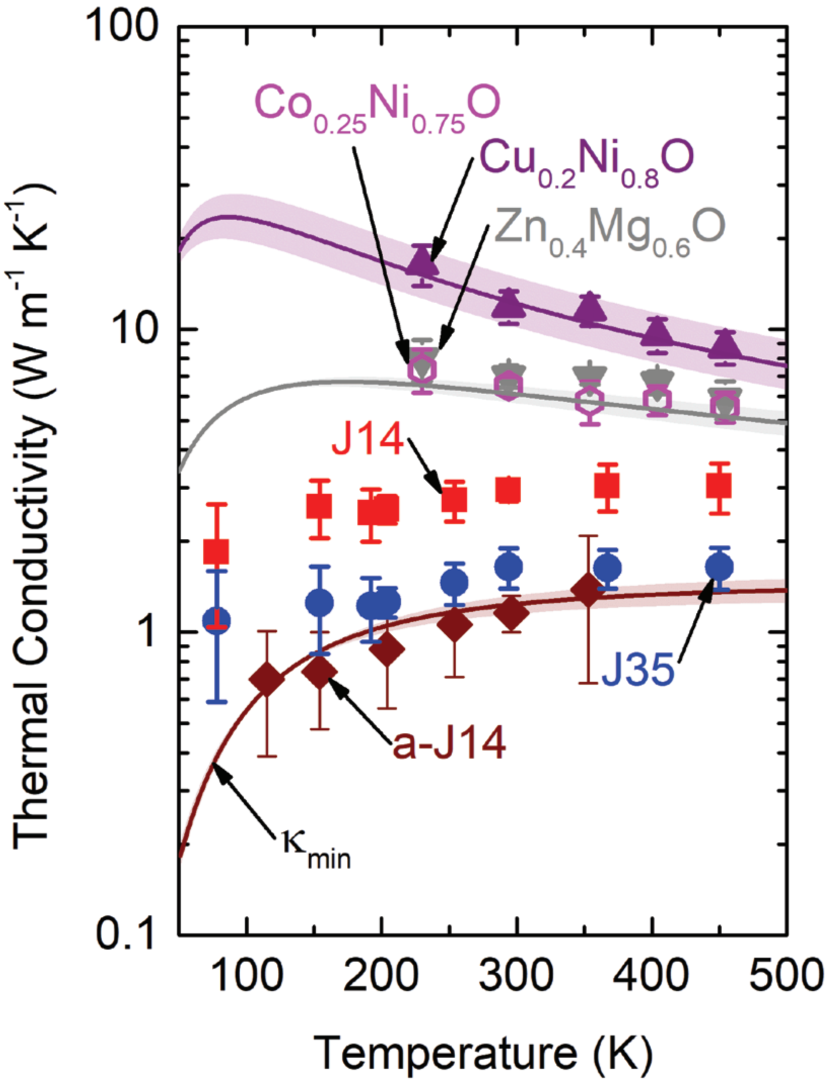


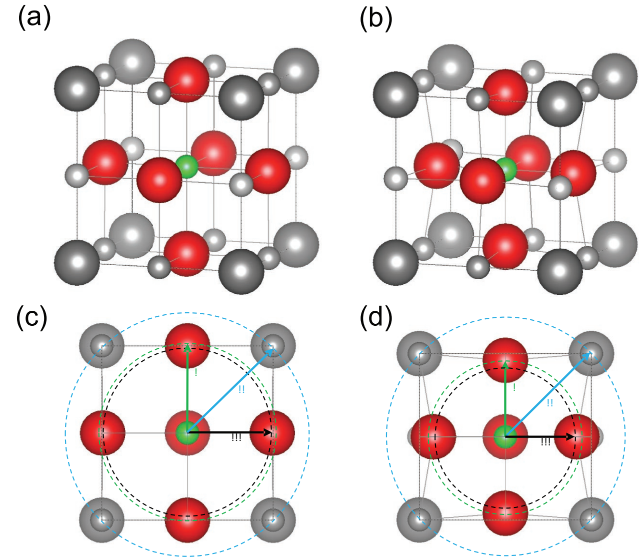


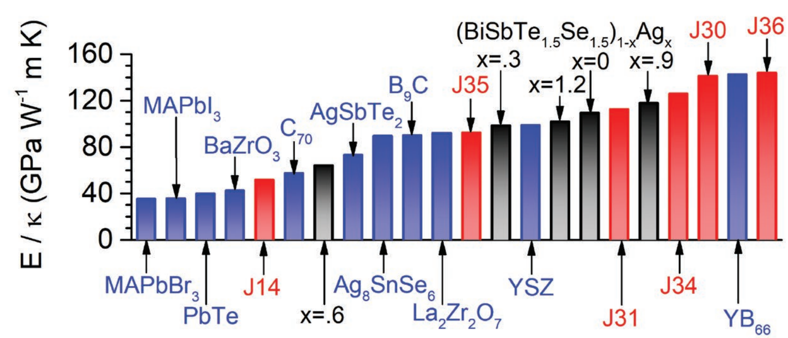


Adv. Mat. **30**, 1805004 (2018)

Ultralow phonon conduction enabled by lattice distortion

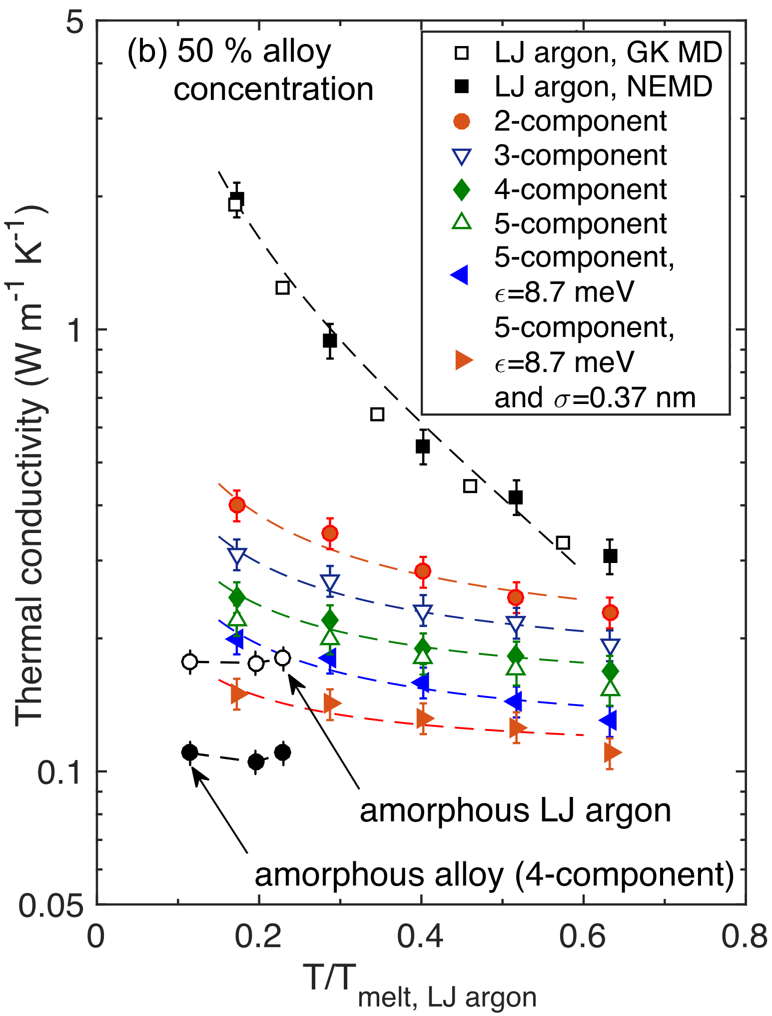


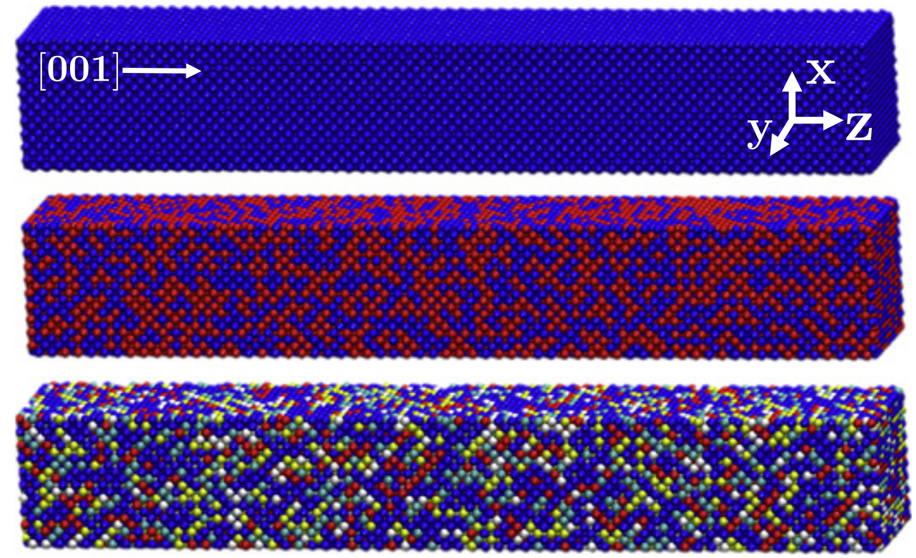


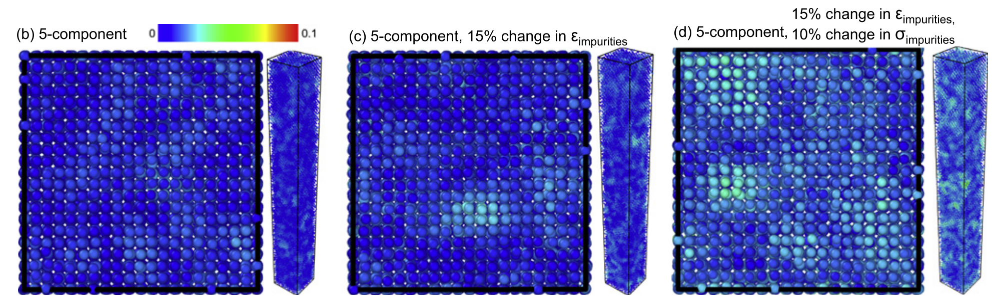


Adv. Mat. **30**, 1805004 (2018)

Ultralow phonon conduction enabled by lattice distortion





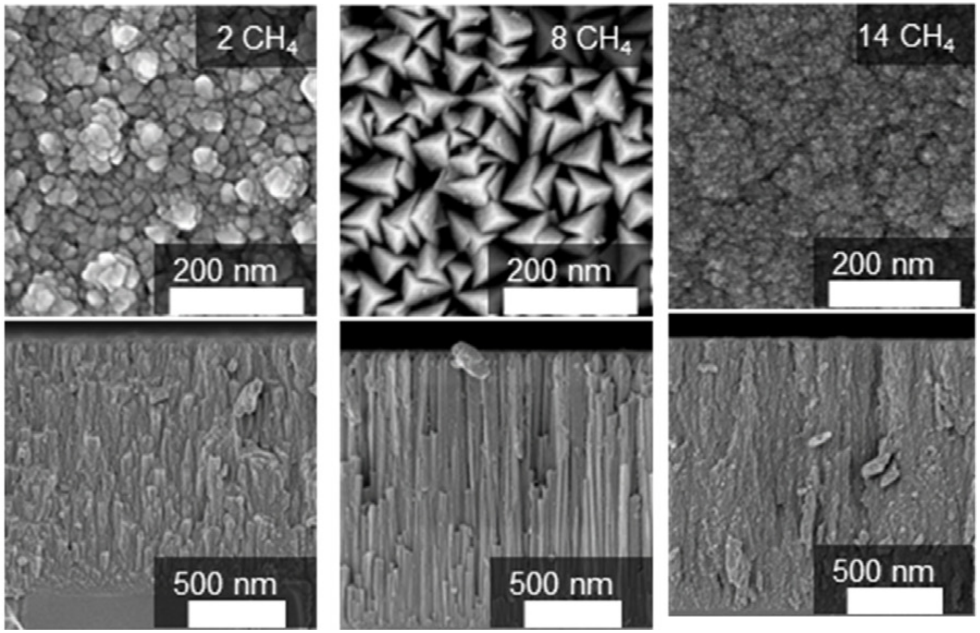


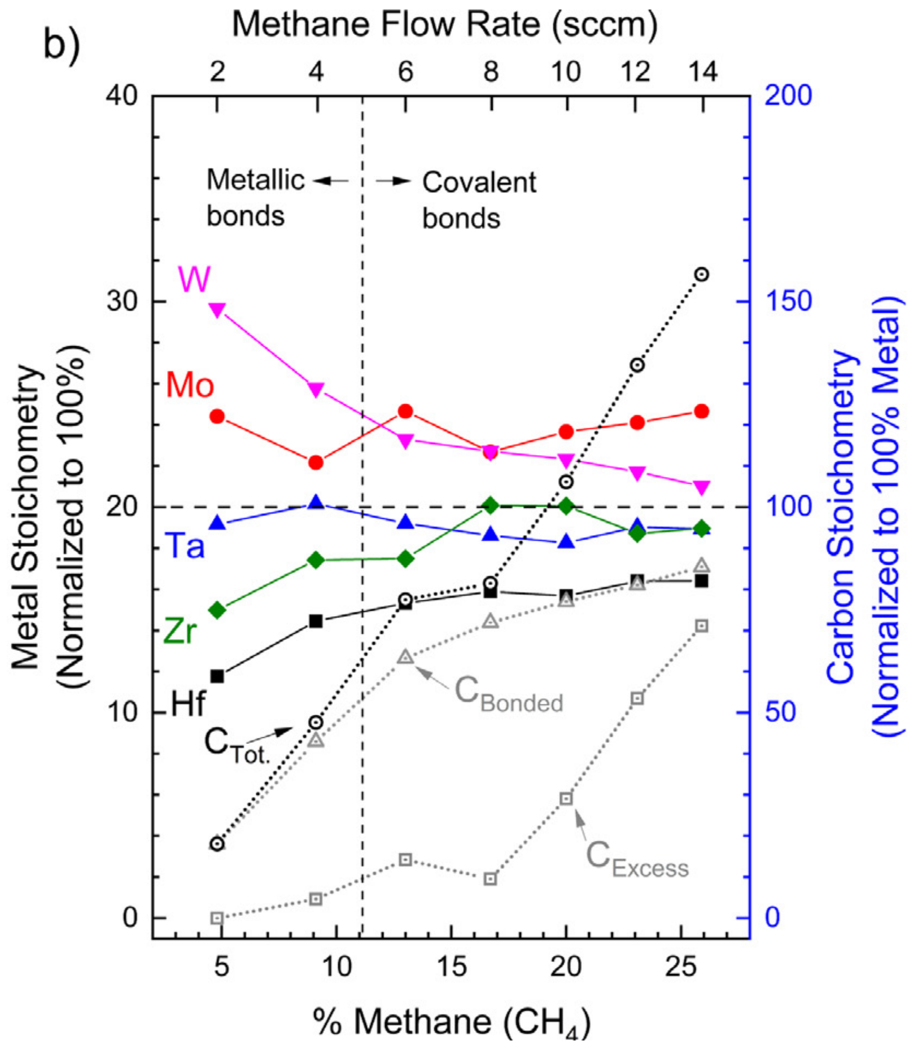
Sctripta Mat. **138**, 134 (2017)

Electron vs. phonon heat conduction in HE ceramics

- Phonon conduction reduced in HE-ceramics due to increased phonon scattering from chemical disorder
- Prior work focused on oxides with no free carriers to contribute to thermal conduction
- What is interplay between electrons and phonons on heat conduction? Study in HE-carbides

HE carbide thin films (JP Maria - PSU)





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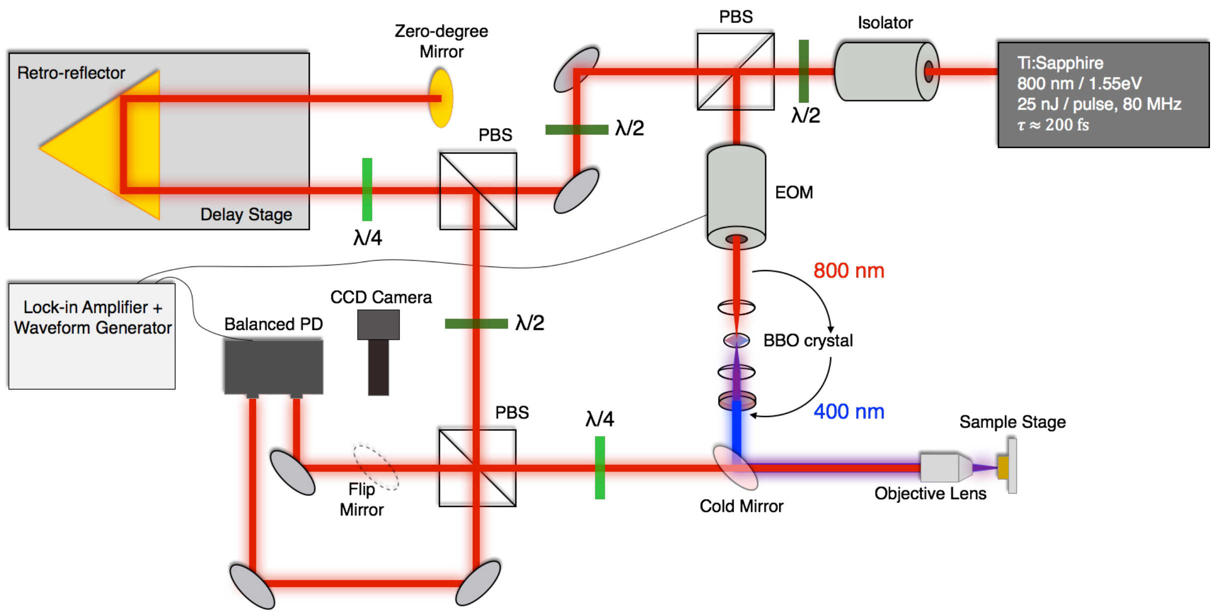
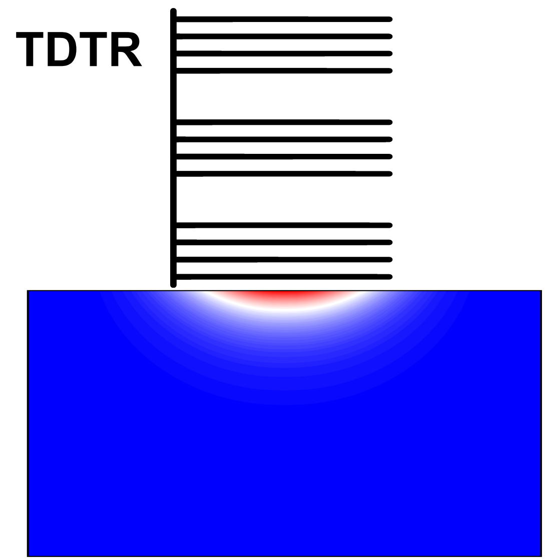
Thermal conductivity measurements – TDTR

Thin film or "near surface" measurements





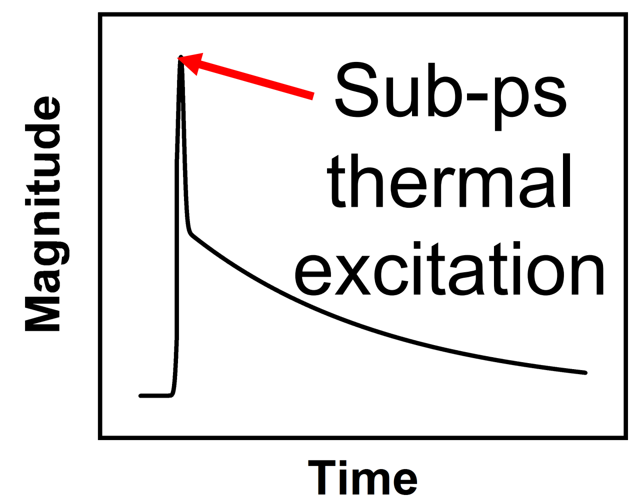
TDTR Reviews and Analyses

Rev. Sci. Instr. **75**, 5119;

Rev. Sci. Instr. **79**, 114902

J. Heat Trans. **132**, 081302;

Ann. Rev. Heat Trans. **16**, 159



Our recent TDTR measurements of the thermal conductivity of HE ceramics: bulk and thin films

Journal of Materiomics 5 (2019) 337–343

Contents lists available at ScienceDirect

Journal of Materiomics

journal homepage: www.journals.elsevier.com/journal-of-materiomics/

A high-entropy silicide: $(Mo_{0.2}Nb_{0.2}Ta_{0.2}Ti_{0.2}W_{0.2})Si_2$

Joshua Gild [a], Jeffrey Braun [b], Kevin Kaufmann [c], Eduardo Marin [c], Tyler Harrington [a], Patrick Hopkins [b], Kenneth Vecchio [a, c], Jian Luo [a, c, *]

Journal of the European Ceramic Society 38 (2018) 3578–3584

Contents lists available at ScienceDirect

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Journal of the European Ceramic Society

journal homepage: www.elsevier.com/locate/jeurceramsoc

Original Article

High-entropy fluorite oxides

Joshua Gild[a], Mojtaba Samiee[b], Jeffrey L. Braun[c], Tyler Harrington[a], Heidy Vega[b], Patrick E. Hopkins[c], Kenneth Vecchio[a,b], Jian Luo[a,b,*]

Ceramics International 46 (2020) 6906–6913

Contents lists available at ScienceDirect

ELSEVIER

Ceramics International

journal homepage: www.elsevier.com/locate/ceramint

Thermal conductivity and hardness of three single-phase high-entropy metal diborides fabricated by borocarbothermal reduction and spark plasma sintering

Joshua Gild[a], Andrew Wright[b], Kathleen Quiambao-Tomko[c], Mingde Qin[a], John A. Tomko[d], Md Shafkat bin Hoque[c], Jeffrey L. Braun[c], Blake Bloomfield[b], Daniel Martinez[b], Tyler Harrington[a], Kenneth Vecchio[a,b], Patrick E. Hopkins[c,d,e], Jian Luo[a,b,*]

COMMUNICATION

ADVANCED MATERIALS

Ceramics

www.advmat.de

Charge-Induced Disorder Controls the Thermal Conductivity of Entropy-Stabilized Oxides

*Jeffrey L. Braun, Christina M. Rost, Mina Lim, Ashutosh Giri, David H. Olson, George N. Kotsonis, Gheorghe Stan, Donald W. Brenner, Jon-Paul Maria, and Patrick E. Hopkins**

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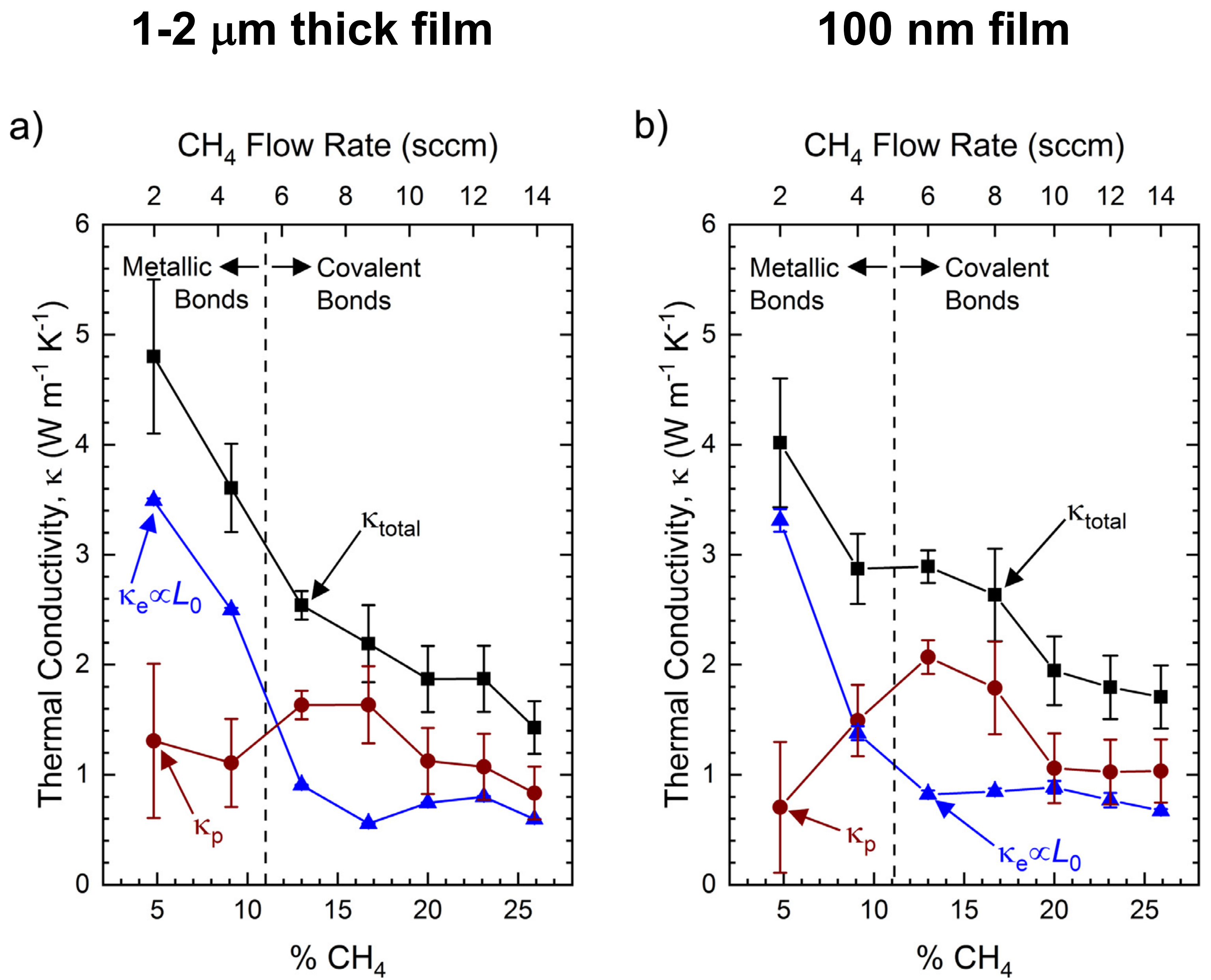
Thermal conductivity of HECs



What what do we assume about κ_e and L?

The Widemann-Franz Law and $L=L_0$

$$\kappa_e = \sigma L T$$

1853. ANNALEN No. 8.

DER PHYSIK UND CHEMIE.

BAND LXXXIX.

I. *Ueber die Wärme-Leitungsfähigkeit der Metalle; von G. Wiedemann und R. Franz.*

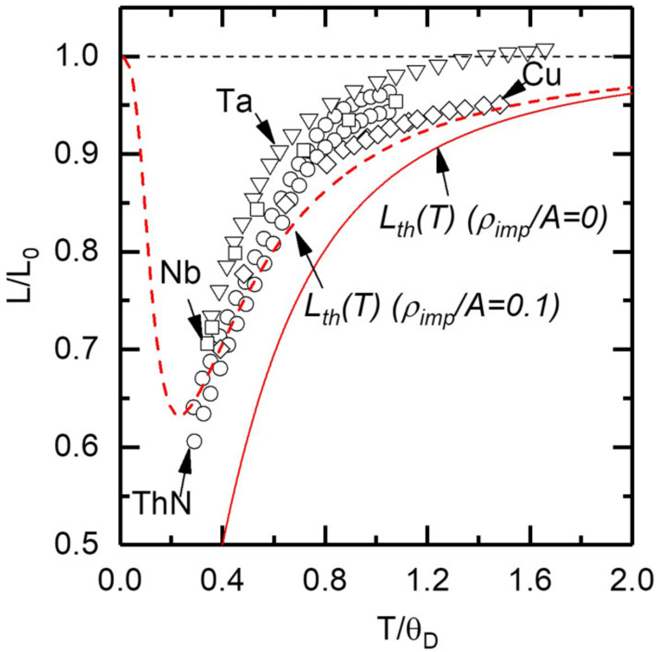
What what do we assume about κ_e and L?

The Wiedemann-Franz Law and $L = L_0$

Only valid at low or high T

Or

If sufficient elastic electron scattering



PHYSICAL REVIEW MATERIALS **1**, 065002 (2017)

Phonon and electron contributions to the thermal conductivity of VN_x epitaxial layers

Qiye Zheng,[1,*] Antonio B. Mei,[1] Mohit Tuteja,[1] Davide G. Sangiovanni,[2,3] Lars Hultman,[3] Ivan Petrov,[1,3] J. E. Greene,[1,3] and David G. Cahill[1]

[1]*Department of Materials Science and Engineering, Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, 104 South Goodwin, Urbana, Illinois 61801, USA*

[2]*Atomistic Modelling and Simulation, ICAMS, Ruhr-Universität Bochum, D-44801 Bochum, Germany*

[3]*Department of Physics (IFM), Linköping University, SE-581 83 Linköping, Sweden*

(Received 25 June 2017; revised manuscript received 9 October 2017; published 20 November 2017)

What what do we assume about κ_e and L_0?

The Wiedemann-Franz Law and *L* more general form

$$L_{\mathrm{th}} = \frac{\rho_{\mathrm{imp}} + \left(\frac{\Theta_D}{T}\right)^5 J_5\left[\frac{\Theta_D}{T}\right]}{\rho_{\mathrm{imp}} + \left(\frac{\Theta_D}{T}\right)^5 J_5\left[\frac{\Theta_D}{T}\right]\left(1 + \frac{3}{\pi^2}\left(\frac{k_F}{q_D}\right)^2\left(\frac{\Theta_D}{T}\right)^2 - \frac{1}{2\pi^2}\frac{J_7\left[\frac{\Theta_D}{T}\right]}{J_5\left[\frac{\Theta_D}{T}\right]}\right)} L_0$$

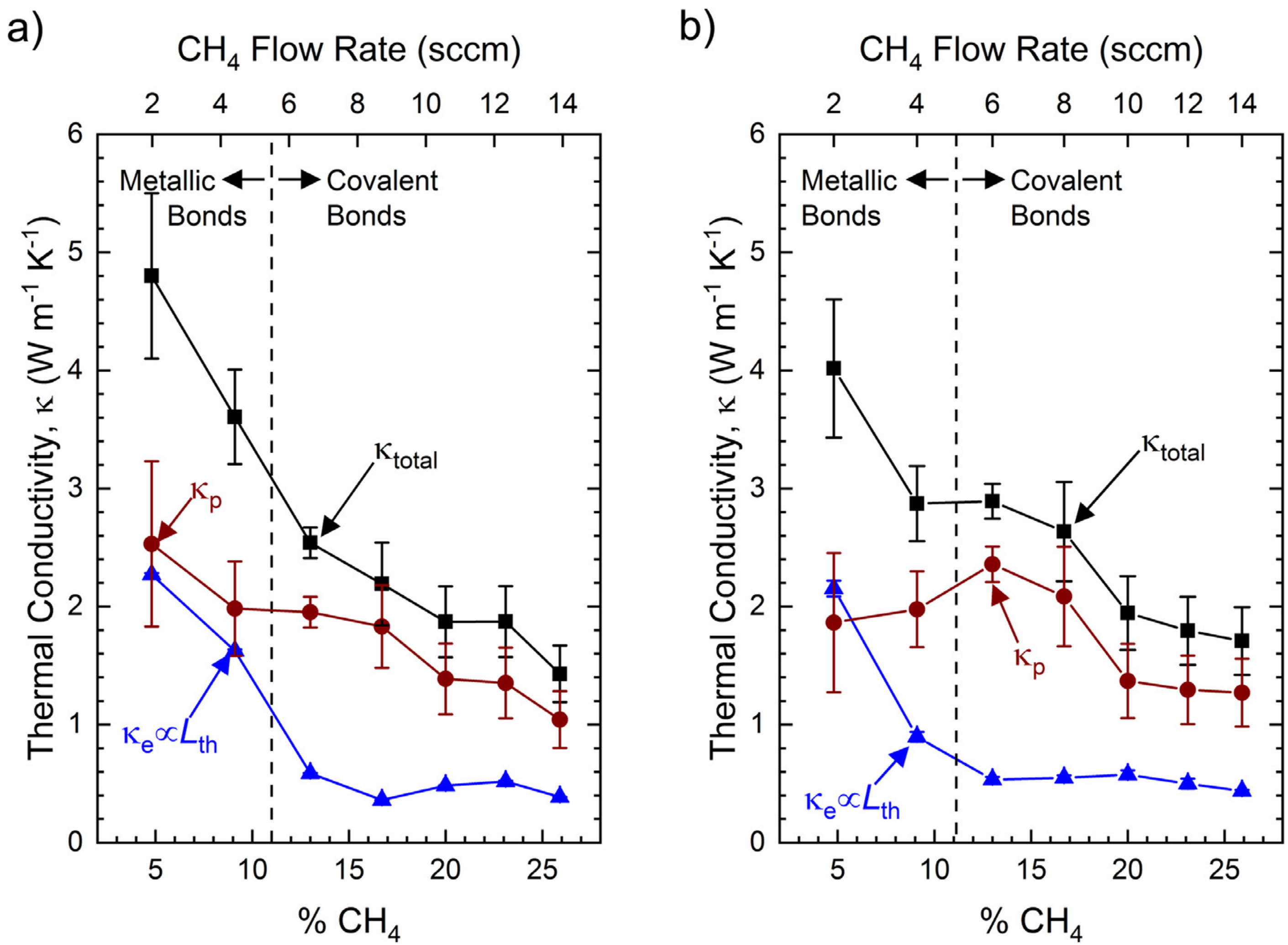
THE THERMAL CONDUCTIVITY OF METALS

BY R. E. B. MAKINSON, St John's College

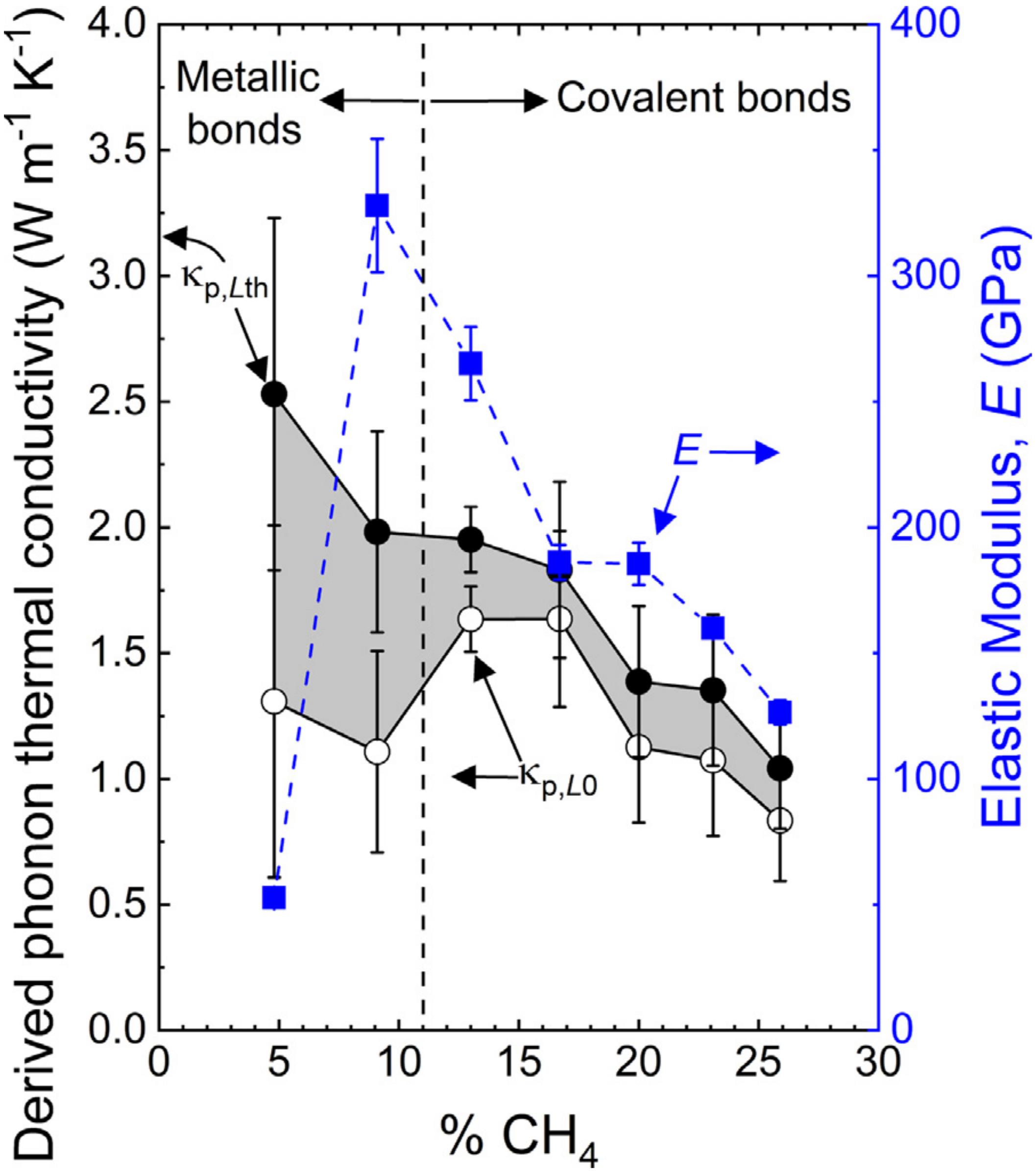
[Communicated by Mr A. H. WILSON]

[*Received* 9 May, *read* 16 May 1938]

Does assumption of *L* change our conclusion about HECs? No



Phonon conductivity of HECs scale with modulus



But only in non-metallic phase

$$\kappa \propto \frac{E}{M_{\mathrm{avg}}}$$

Summary: Carbon content dictates electron and phonon thermal conductivity in high entropy ceramics through both electron thermal conductivity changes and modulus changes

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