An Investigation into the Effects of Interface Stress and Interfacial Arrangement on Temperature Dependent Thermal Properties of a Biological and a Biomimetic Material

Final Technical Report

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DISCLAIMER

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EXECUTIVE SUMMARY

A significant effort in the biomimetic materials research is on developing materials that can mimic and function in the same way as biological tissues, on bio-inspired electronic circuits, on bio-inspired flight structures, on bio-mimetic materials processing, and on structural biomimetic materials, etc. Most structural biological and biomimetic material properties are affected by two primary factors: **(1)** interfacial interactions between an organic and an inorganic phase usually in the form of interactions between an inorganic mineral phase and organic protein network; and **(2)** structural arrangement of the constituents. Examples are exoskeleton structures such as spicule, nacre, and crustacean exoskeletons. A significant effort is being directed towards making synthetic biomimetic materials based on a manipulation of the above two primary factors. The proposed research is based on a hypothesis that in synthetic materials with biomimetic morphology thermal conductivity, *k*, (how fast heat is carried away) and thermal diffusivity, *D*, (how fast a material's temperature rises: proportional to the ratio of *k* and heat capacity) can be engineered to be either significantly low or significantly high based on a combination of chosen interface orientation and interfacial arrangement in comparison to conventional material microstructures with the same phases and phase volume fractions.

METHOD DEVELOPMENT

1. We have established a combined Raman spectroscopy and nanomechanical loading based experimental framework to perform environment (liquid vs. air vs. vacuum) dependent and temperature dependent (~1000 degree-C) *in-situ* thermal diffusivity measurements in biomaterials at nanoscale to micron scale along with the corresponding analytical theoretic calculations. (Zhang and Tomar, 2013)
2. We have also established a new classical molecular simulation based framework to measure thermal diffusivity in biomolecular interfaces. We are writing a publication currently (Qu and Tomar, 2013) to report the framework and findings in tropocollagen-hydroxyapatite based idealized biomaterial interfaces.

PHYSICAL FINDINGS

1. Analyses using experiments have revealed that in the case of bone thermal conductivity and thermal diffusivity at micron scale shows significant dependence on compressive stress and temperature. Overall, there is a decrease with respect to increase in temperature and increase with respect to increase in compressive stress. Bio-molecular simulations on idealized tropocollagen-hydroxyapatite interfaces confirm such findings. However, simulations also reveal that thermal diffusivity and thermal conductivity can be significantly tailored by interfacial orientation. More importantly, in inorganic materials, interfaces contribute to reduce thermal conductivity and diffusivity. However, analyses here reveal that both can be increased despite presence of a lot of interfaces.
2. Based on significant role played by interfaces in affecting bone thermal properties, a crustacean-exoskeleton system is examined for thermal diffusivity using the newly developed setup. Special emphasis here is on this system since such arrangement is found to be common in fresh water shrimp as well as in some deep water organisms surviving in environment extremes. Experiments reveal that in such system thermal diffusivity is highly tailorable.
3. Overall, experiments and models have established that in biomaterial interfaces a counterintuitive role of interfaces in mediating thermal conduction as a function of stress and temperature is possible in contrast to inorganic materials where interfaces almost always lead to reduction of thermal conductivity as a function of such factors. More investigations are underway to reveal physical origins of such counter-physical characteristics. Such principles can be significantly useful in developing new and innovative bioenergy and inorganic energy systems where heat dissipation significantly affects system performance.

Description of Findings

The following are the main findings of the ongoing research project.

Method Development

3. We have established a combined Raman spectroscopy and nanomechanical loading based experimental framework to perform environment (liquid vs. air vs. vacuum) dependent and temperature dependent (~1000 degree-C) *in-situ* thermal diffusivity measurements in biomaterials at nanoscale to micron scale along with the corresponding analytical theoretic calculations. (Zhang and Tomar, 2013)
4. We have also established a new classical molecular simulation based framework to measure thermal diffusivity in biomolecular interfaces. We are writing a publication currently (Qu and Tomar, 2013) to report the framework and findings in tropocollagen-hydroxyapatite based idealized biomaterial interfaces.

Physical Findings

4. Analyses using experiments have revealed that in the case of bone thermal conductivity and thermal diffusivity at micron scale shows significant dependence on compressive stress and temperature. Overall, there is a decrease with respect to increase in temperature and increase with respect to increase in compressive stress. Bio-molecular simulations on idealized tropocollagen-hydroxyapatite interfaces confirm such findings. However, simulations also reveal that thermal diffusivity and thermal conductivity can be significantly tailored by interfacial orientation. More importantly, in inorganic materials, interfaces contribute to reduce thermal conductivity and diffusivity. However, analyses here reveal that both can be increased despite presence of a lot of interfaces.
5. Based on significant role played by interfaces in affecting bone thermal properties, a crustacean-exoskeleton system is examined for thermal diffusivity using the newly developed setup. Special emphasis here is on this system since such arrangement is found to be common in fresh water shrimp as well as in some deep water organisms surviving in environment extremes. Experiments reveal that in such system thermal diffusivity is highly tailorable. More importantly, experiments show that in such materials thermal diffusivity shows an increase as a function of temperature increase contrary to the normal notion in inorganic materials where presence of interfaces leads to reduction in thermal conductivity and consequently thermal diffusivity.
6. Overall, experiments and models have established that in biomaterial interfaces a counterintuitive role of interfaces in mediating thermal conduction as a function of stress and temperature is possible in contrast to inorganic materials where interfaces almost always lead to reduction of thermal conductivity as a function of such factors. More investigations are underway to reveal physical origins of such counter-physical characteristics. Such principles can be significantly useful in developing new and innovative bioenergy and inorganic energy systems where heat dissipation significantly affects system performance.

Students Who Worked on the Project:

Yang Zhang (Experiments) and Tao Qu (modeling).. Both were supported full time during this period.

Publications (supported by DoE-BES with no cross-connection with another funding agency):

1. Zhang, Y., Gan, M., and Tomar, V., 2014, "Raman Thermometry Based Thermal Conductivity Measurement of Bovine Cortical Bone as a Function of Compressive Stress", Journal of Nanotechnology in Engineering and Medicine, May 2014, Vol. 5, 021003 (11 pages)
2. Qu, T., and Tomar, V., 2014, "An Analysis of the Effects of Temperature and Structural Arrangements on the Thermal Conductivity and Thermal Diffusivity of Tropocollagen-Hydroxyapatite Interfaces", Material Science and Engineering-C, vol. 38, pp 28-38

Publications (co-shared with other grants):

1. Tao Qu, Devendra Verma, Vikas Tomar, Mehran Shahidi, Bernhard Pichler, Christian Hellmich, 2015, “Mechanics of Organic-Inorganic Bio-Interfaces – implications for strength and creep properties” (to appear in Material Research Society Bulletin 2015 April issue)
2. Tao Qu, Devendra Verma, Milad Alucozai and Vikas Tomar, 2015, “Influence of Interfacial Interactions on Deformation Mechanism and Interface Viscosity in Chitin-Calcite Interfaces” (submitted to Acta Biomaterialia)

Invited Talks:

1. Qu, T., Zhang, Y. and Tomar, V., 2013, “Interfacial Biothermomechanics of BioMaterial Interfaces”, MRS Fall meeting 2013
2. Qu, T., Zhang, Y. and Tomar, V., 2013, “Interfacial Biomechanics Of Material Interfaces in Tropocollagen and Chitin Based Materials”, Thermec Meeting, December 2013

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