

# New Horizons for Mechanical Spectroscopy in Materials Science

NICOLÁS MUJICA,<sup>1</sup> MICHAEL DEMKOWICZ,<sup>2</sup> FERNANDO LUND,<sup>1,4</sup>  
and ALFREDO CARO<sup>3</sup>

1.—Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago, Chile. 2.—Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA. 3.—Materials Science and Technology Division, Los Alamos National Laboratory, Los Alamos, NM 87544, USA. 4.—e-mail: flund@cimat.cl

Mechanical spectroscopy investigates materials behavior using acoustic techniques. This technique saw its heyday in the 1960s and 1970s, but recent advances in measurement, modeling, and characterization open up new possibilities in this field. Novel techniques such as resonant ultrasound spectroscopy (RUS) and atomic force microscopy (AFM)-based local acoustic measurements enable high-precision investigations of previously inaccessible phenomena. Atomistic and mesoscale modeling, high-resolution microscopy, and modern microstructure characterization methods offer new approaches for interpreting acoustic data. Judicious integration of measurement, modeling, and characterization may transform classic mechanical spectroscopy into a powerful tool for investigating the micromechanisms of materials behavior.

The international symposium “New Horizons for Mechanical Spectroscopy in Materials Science” was held at the TMS 2015 Annual Meeting and Exhibition with the aim of addressing emerging opportunities for applications of mechanical spectroscopy in materials science. Emphasis was given to new mechanical spectroscopy techniques, integration of mechanical spectroscopy with materials modeling, and applications to complex solids.

Several exciting recent developments were reported at this symposium. For instance, the notion of defects in crystalline structures is easy to grasp; but is it possible to define a defect in a material that has no long-range order such as a glass? This question has been explored numerically, using molecular dynamics, and experimentally. Whatever the exact nature of hypothesized defects in

amorphous solids, they should interact with acoustic waves. Thus, mechanical spectroscopy provides a nonintrusive way of ascertaining their properties. In this topic, M. Atzmon presented results about the role of shear transformation zones on the dynamical response of glasses, and L. Huang explained the use of Raman and Brillouin scattering to understand the behavior of glasses under extreme conditions.

Another topic was the use of *ab initio* numerical codes or multimillion atom classic potential simulations to explore the effect that defects have on macroscopic acoustic response of crystalline solids. E. Bitzek showed results on the dynamics of dislocations at high velocities using molecular dynamics, and E. Clouet used quantum mechanical codes to shed new light on the internal friction behavior of irradiated zirconium.

A third example concerned the mechanical behavior of surfaces, thin films, and interfaces, all of which might be interrogated both through atomistic numerical simulation and elastic waves. This topic was highlighted by the talk of R. Schwarz, who showed how to use Rayleigh waves to study metal-metal interfaces.

Resonant ultrasound spectroscopy, in which the normal modes of vibration of a material provide information about its microstructure, has evolved into an amazingly accurate technique that can explore many different phenomena through their coupling to the material strain. A. Migliori gave an overview of the current capacities of this technique, M. Hirao showed how it can be used to explore the local variation of the elastic constants of a material, and M. Carpenter provided results on a variety of materials behavior near a phase transition. In the related field of laser ultrasonics, D. Hurley provided measurements of local elastic properties of nuclear fuel surrogates.

Michael Demkowicz is the guest editor for the Chemistry and Physics of Materials Committee, a joint committee of the TMS Functional Materials Division (FMD) and the TMS Structural Metals Division (SMD); and coordinator of the topic New Horizons in Mechanical Spectroscopy in this issue.

Finally, metamaterials, or materials made of building blocks that are not atoms or molecules but macroscopic structures, such as nylon lines, have opened up a whole new field in which objects that once were the realm of science fiction, such as the perfect acoustic absorber, are no longer a dream. J. Page gave a talk about phononic crystals, and M. Moleron discussed acoustic lenses.

This special topic of *JOM* presents four illustrative articles that highlight potential new directions for the mechanical spectroscopy in materials science. They also show the diversity of topics covered at the TMS 2015 symposium.

The paper by A. Tanguy, "Vibrational Modes and Characteristic Length Scales in Amorphous Materials," illustrates how atomic-level modeling can be used to investigate the acoustic behavior of amorphous solids. Such materials have no crystalline order and, as a result, exhibit markedly different acoustic properties from crystalline solids. Tanguy shows that these properties might be related to the local heterogeneity of amorphous materials. Examples of such heterogeneity include variable, location-dependent stiffness and density. Atomic configurations that are nearly unstable and likely to undergo a shear transformation (giving rise to plasticity) also might have characteristic acoustic signatures. These atomic-level heterogeneities occur over characteristic length scales that, in turn, are reflected in phonon mode shapes and may be probed with spectroscopic measurements.

M.P. Short et al., in "Applications of Transient Grating Spectroscopy to Radiation Materials Science," discuss applications of mechanical spectroscopy to characterizing property and structure evolution in solids under irradiation. They motivate their discussion with the need for rapid, nondestructive, and noncontact methods of interrogating radiation damage in components used in nuclear energy. After reviewing a range of approaches used in the past, Short et al. focus in on one promising method: laser-wave surface acoustic wave (LSAW) analysis. This technique has the potential to extract information concerning elastic constants and thermal conductivity as well as to identify the onset of self-organization of radiation defects. Variations of these physical properties with irradiation dose could provide a means of inferring the internal, radiation-induced evolution of microstructure.

In the paper "Review on Acoustic Transducers for Resonant Ultrasound Spectroscopy," Nakamura et al. review several ultrasonic transduction methods that are used for resonant ultrasound spectroscopy, which allows the precise determination of elastic constants of materials. The selected methods are mode-selective electromagnetic acoustic resonance, tripod piezoelectric transducer coupled with a laser-Doppler interferometer, and antenna transmission acoustic resonance. The authors discuss the main aspects of these techniques and show their complementarity and advantages with respect to

the traditional resonant ultrasonic spectroscopy. For example, the study shows how the antenna method can be used for the mapping of the effective Young's modulus on small surfaces (resonant ultrasound microscope [RUM]).

"Use of Ultrasound to Measure Dislocation Density," by Barra et al., presents a review of the use of ultrasound (US) technology as a powerful, nonintrusive tool for the measurement of dislocation density in materials. Dislocations are responsible for the plastic behavior of crystalline materials, but their proper experimental characterization is very difficult. This paper first summarizes current standard techniques, such as x-ray diffraction (XRD) and transmission electron microscopy (TEM), which are intrusive and make strong assumptions. Then, the authors present recent theoretical developments in the study of elastic wave interactions with dislocations and the effect on coherent acoustic wave propagation. Finally, experimental results that support the theoretical picture are presented, showing that US is a promising method for the characterization of plasticity in materials.

To conclude, it is possible to say that experimentally, in addition to the increasing power of microscopy analysis, there is a clear trend to develop nonintrusive and precise measurement techniques using ultrasonic waves, either for the characterization of surfaces, thin films, or bulk samples. Although mechanical spectroscopy as practiced in the 1960s and 1970s was mostly an observational science, marked progress in computational power, both for analyzing experimental data and solving numerical models, gives us today the possibility of relating each experimental observation to particular properties of defects at the atomic scale. These developments truly open new horizons for mechanical spectroscopy, as was clearly shown in the TMS 2015 symposium.

The following articles being published under the topic of New Horizons in Mechanical Spectroscopy provide excellent details and research on the subject. To download any of the papers, follow the URL <http://link.springer.com/journal/11837/67/8/page/1> to the table of contents page for the August 2015 issue (vol. 67, no. 8).

- "Vibrational Modes and Characteristic Length Scales in Amorphous Materials," by Anne Tanguy
- "Applications of Transient Grating Spectroscopy to Radiation Materials Science," by Michael P. Short, Cody A. Dennett, Sara E. Ferry, Yang Yang, Vikash K. Mishra, Jeffrey K. Eliason, Alejandro Vega-Flick, Alexei A. Maznev, and Keith A. Nelson
- "Review on Acoustic Transducers for Resonant Ultrasound Spectroscopy," by N. Nakamura, H. Ogi, and M. Hirao
- "Use of Ultrasound to Measure Dislocation Density," by Felipe Barra, Rodrigo Espinoza-González, Henry Fernández, Fernando Lund, Agnès Maurel, and Vincent Pagneux