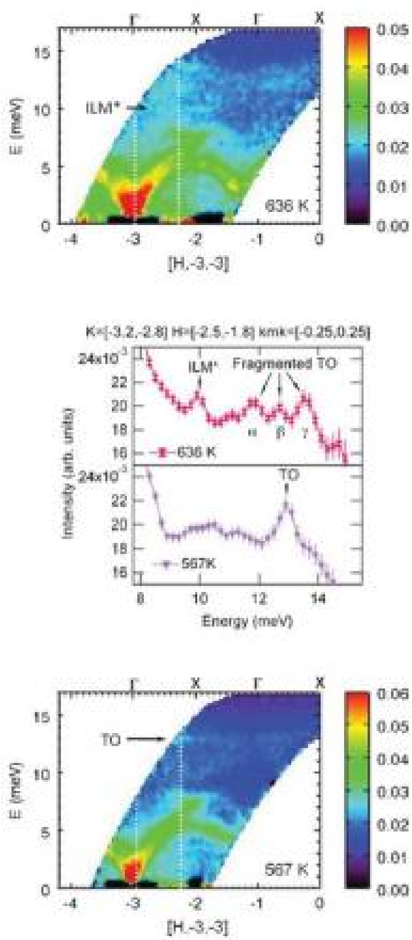
Startling thermal energy behavior revealed by neutron scattering

June 22 2011, by Deborah Counce



Data from ARCS show that, with a small increase in temperature, a new feature in the scattering from NaI appears, indicating that localized energy modes (ILMs) are present. The wide coverage of the instrument allowed the interaction of these new modes with other atomic vibrations to be studied, revealing the novel dynamical nature of the patterns within the unchanged crystal structure.

(PhysOrg.com) -- A discovery by researchers working at the Spallation Neutron Source upends long held assumptions about the microscopic behavior of materials in an equilibrium condition. The findings could influence further research in advanced materials, communication and optical systems, and thermoelectric materials that use differences in temperature to produce electricity.

The researchers at the Oak Ridge National Laboratory neutron science facility found that the thermal energy in a crystal at thermal equilibrium (i.e., a state in which the thermal energy is uniformly distributed across the crystal structure) organizes itself into dynamical patterns that are not associated with corresponding changes in the structure of the crystal.

This is the first observation of dynamical patterns of ILMs in a material in thermal equilibrium and the first in an atomic lattice. The new results "extend the notion of complex energy self-organization to equilibrium processes and down to the scale of atoms," noted principal investigator Mike Manley of Lawrence Livermore National Laboratory.

Beyond the contribution to theory, the insights are of great practical importance because they appeared under conditions ordinary in the world of material applications, he said. "It's a fundamental new understanding of properties occurring at the temperatures at which we use materials."

Scientific Reports, a new online publication from Nature Publishing Group, published the findings in its June 14 issue (available with open access at www.nature.com/srep/2011/11061 … /full/srep00004.html). The experiments were conducted on ARCS, the Wide Angular-Range Chopper Spectrometer at the SNS. Research team members are from Lawrence Livermore and Oak Ridge national labs and Cornell University.

The thermal energy in an ordinary crystal exists mainly in the form of tiny atomic vibrations that ripple in waves through the material. It might seem that in a crystal at equilibrium, these waves would emanate symmetrically and uniformly in all directions, much as ripples spread from a stone thrown into a calm pool. But physicists have realized for decades that some thermal energy in a material can actually collect in discrete packets, called intrinsic localized modes (ILMs) that break the symmetry of the crystal.

Scientists have assumed that ILMs formed randomly throughout a crystal in equilibrium. However, as the researchers analyzed their ARCS data, they realized that the ILMs were emerging according to a regular pattern, said Manley. At temperatures between 614 and 636 K, the ILMs in the crystal began switching as a unit back and forth between one pattern and another. Then as the temperature of the sample rose beyond 636 K, they returned to their original pattern. "This pattern isn't something we would have tried to look for specifically, because we didn't expect it. But as we were piecing together the data, we saw the whole pattern and we saw that the ILMs weren't random, Manley said."

Another surprise was that the crystal structure didn't change along with the dynamics as the ILMs organized: the ILMs organized themselves in complex, shifting dynamical patterns even as the crystal lattice remained unchanged. Localized packets of energy in the crystal had decoupled from the rest of the lattice and were vibrating differently from it.

"If you look at the crystal structure, you see nothing happening. It's unchanged. But if you could stick your head inside the crystal, at the atomic scale, you would see every third atom moving in a way that's different from the two atoms next to them," said Manley. "We assume atoms that are identical all vibrate the same way. But this experiment showed some of the atoms vibrating differently although they're not structurally different," he said. Such behavior of self-organizing energy is common in nature, he said, but only in nonequilibrium situations in which some force is driving energy across a system—for example, cloud formation and whirlpools driven by convective energy flow.

The research team went into the experiment expecting to find ILMs in NaI, Manley said. They thought ILMs would appear smoothly with increasing temperature. But instead, the ILMs seemed to fade out at a certain temperature and then reappear at another temperature. The capabilities of SNS and ARCS made it possible to collect the fine detail needed to resolve what the scientists were seeing, he noted. "We looked at it with a new tool that could really see in detail and get a much more complete view in reciprocal space, in four dimensions—the three spatial directions plus frequency—and we saw this pattern. We wouldn't have been able to see the pattern if SNS and ARCS hadn't been available. We never could have collected that much data at all those temperatures otherwise. SNS gave us the capability to see the whole thing."

Manley said he wants to pursue the research in other materials and under a broader range of conditions. Other ordered states of energy may occur outside the fairly narrow range of temperatures the ARCs experiment explored, and new patterns may emerge. Practical applications often arise from the type of complexity the experiment revealed. "This will change our perspective; it will lead to applications; it will inform theory," he said.

Provided by Oak Ridge National Laboratory

Citation: Startling thermal energy behavior revealed by neutron scattering (2011, June 22) retrieved 26 April 2024 from
https://phys.org/news/2011-06-startling-thermal-energy-behavior-revealed.html