Materials science

Characterizing atomic orbitals

Pulses of corkscrew-like X-rays prove useful for probing the properties of atomic orbitals

The properties of a solid material depend on the behaviour of its electrons: some electrons are localized near the nucleus, whereas others travel throughout the crystal lattice. Researchers at Japan's NAIST have now shown that an unusual property of electromagnetic radiation can provide previously unavailable information on these valence band electrons, enabling more detailed material characterization[1].

An atom is made up a nucleus surrounded by electrons. The outermost electrons, or valence electrons, largely determine how an atom interacts with molecules and other atoms. So it is important to fully understand the properties of these electrons.

"Copper is nonmagnetic, whereas nickel, which has one less electron than copper, is ferromagnetic," says NAIST researcher Fumihiko Matsui. "If we can selectively excite a valence electron, then we can explore the behaviour of key atomic orbitals responsible for these electronic properties."

To achieve this, Matsui and his colleagues from NAIST's Green Nanosystem Laboratory and the Japan Synchrotron Radiation Research Institute have applied their original method called atomic stereography. In this technique, X-ray pulses provide the energy needed for an electron near the core of an atom to escape from its nucleus. The X-rays used by the team have a property known as angular momentum, which gives them a corkscrew-like shape. This angular momentum is transferred to the escaping photoelectron. By measuring the kinetic energy and emission angle of these photoelectrons, the researchers can build a 'stereograph' of the atomic arrangement around the excited atom.

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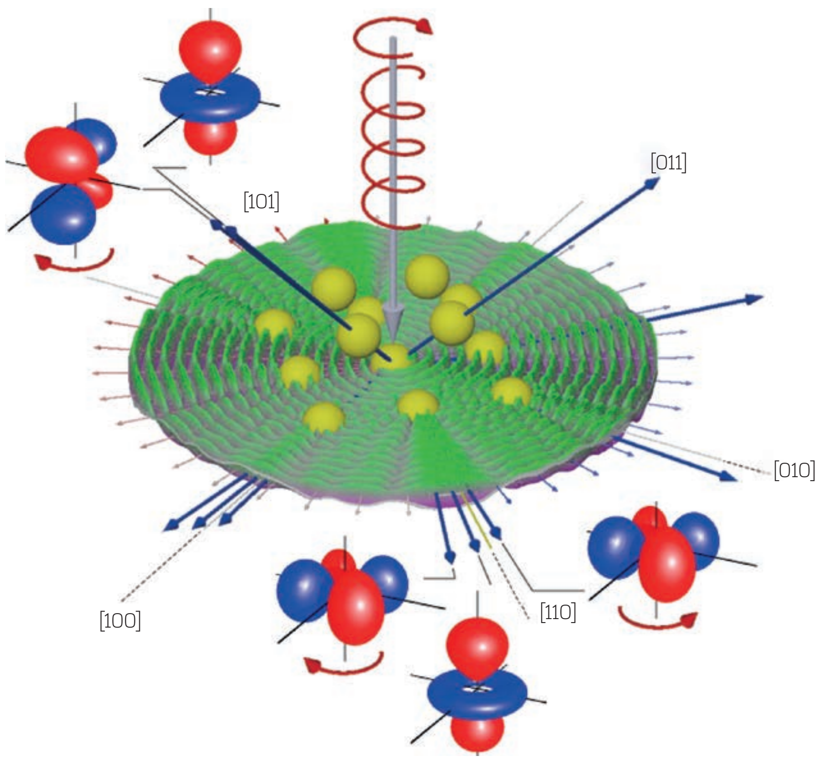
Further electrons, known as Auger electrons, can also escape from the atom as the electrons shuffle around to fill the gap left at the core. Measuring the energy of these Auger electrons can provide further information about the material's electronic structure. Matsui and his co-workers have now shown that, contrary to expectation, Auger electrons can also have angular momentum.

Matsui's team fired a corkscrew-like beam of X-rays at a copper sample and measured the angular distribution of the emitted Auger electrons. From these maps, they were able to identify the non-negligible circular properties of the Auger electron. This observation suggests that the hole left behind by the photoexcited core electron is slightly angular-momentum polarized, which is then passed on to the Auger electron.

"Our aim is to take out valence electrons from a crystal surface and study the property of the newly created excited state," says Matsui. "By combining Auger electron measurement and atomic stereography, we have developed a new technology that enables such physics."



Corkscrew-like X-rays (red) enable electrons to escape from the surface of copper at various angles.

Reference

1. Matsui, F., Fujita, M., Ohta, T., Maejima, N., Matsui, H. *et al.* Selective detection of angular-momentum-polarized Auger electrons by atomic stereography. *Physical Review Letters* **114**, 015501 (2015).

More information about the group's research can be found at the Green Nanosystem Laboratory webpage:
http://mswebs.naist.jp/LABs/matui/index-e.html