Charge Density Waves in Ultrathin Films – Dimensional and Confinement Effects

T.-C. Chiang (江台章)
Department of Physics and Frederick Seitz Materials Research Laboratory, University of Illinois at Urbana-Champaign, Urbana, Illinois, 61801, USA
Department of Physics, National Taiwan University
Department of Physics, National Tsing Hua University

Films as thin as a single molecular layer can exhibit novel properties that are very different from the bulk counterparts. For an illustration, this talk focuses on a model system: titanium diselenide (TiSe2). This material belongs to a vast family of transitional metal dichalcogenides, many of which show charge density wave (CDW) transitions at low temperatures. The CDW order can compete or entangle with other transitions such as superconductivity and antiferromagnetism, and it is a basic phenomenon of great interest in solid state physics. Specifically, $TiSe_2$, with a simple (2x2x2) CDW transition at T_C ~205 K in the bulk, remains a fascinating case. The transition has been attributed variably to excitonic interactions, band-type Jahn-Teller effects, etc. A detailed investigation of the electronic structure is complicated by the three-dimensional nature of the CDW order. The perpendicular electronic momentum is not necessarily conserved in angle-resolved photoemission spectroscopy (ARPES) measurements, making it difficult to pinpoint the gap locations in the Brillouin zone. A single layer of $TiSe_2$, by contrast, has a much simpler two-dimensional electronic band structure. Experimentally, it exhibits a (2x2) CDW transition at T_C = ~232 K, which is, perhaps surprisingly, higher than the bulk T_C. The question is – why? Our measurements of the single layer reveal a small absolute band gap at room temperature, which grows wider with decreasing temperature T below T_C in accordance with a BCS-like mean-field behavior. The corresponding atomic displacements, determined by synchrotron x-ray diffraction, also follow a BCS-like mean-field behavior. The results taken from the single layer, multilayers, and bulk crystals, rationalized by first-principles calculations, provide some detailed answers to long standing questions about CDW physics and associated dimensional effects.

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