FYSM30: Simple, explicit simulations toward a better understanding of nanowires

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Nanowires are thin structures just some billionths of a metre in scale - that's only tens of atoms thick - among the smallest stable structures that current science predicts are possible to create. Made from a variety of materials, nanowires are 'grown' either upright on or built in to a surface using a variety of complicated and challenging means. The way they are made and the materials they are made from naturally control the properties of a nanowire, making its electrical and optical qualities suited to one purpose or another.

Although nanowires have not yet found major commercial or industrial use, their invention being only about two decades old, the unique properties granted by their small size have shown promise in a variety of fields, from simply scaled-down versions of larger devices to new tools made possible by their singular characteristics. Because their high surface area makes nanowires extremely sensitive to surrounding material, they can be used to detect gases and other chemicals. Their electrical properties are being optimized with the goal of being viable to use in solar panels, and they may one day be an integral part of our computer chips. Even the quantum properties resulting from their small size are being used in research. All of this, of course, requires the foundation of solid grasp on the properties of nanowires.

In my project, individual nanowires were simulated on a scale near that of the individual atom, allowing direct control over the shape and properties of the nanowire. The simplicity of the simulation allowed me to simply relate useful electrical properties of nanowires with small changes in their structure. Surface roughness was created by manually changing the shape of the wire, charge simulated by directly putting charges onto or into the wire. This direct method of simulation allows you to easily see the effect of the unavoidable imperfections inherent in the nano-scale This helps to understand them when you see them and to account for them when you cannot control them.

Nanowires are starting to see more use in different fields, as the base of understanding grows and production methods become more certain. But more work is still needed for them to see more widespread use. Knowing how small changes in a nanowire can affect its properties can help people working on new manufacturing methods or designing a nanowire for a particular purpose; my projects aims to help provide such information.