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CONNECTING THE COMPOUND SEMICONDUCTOR COMMUNITY

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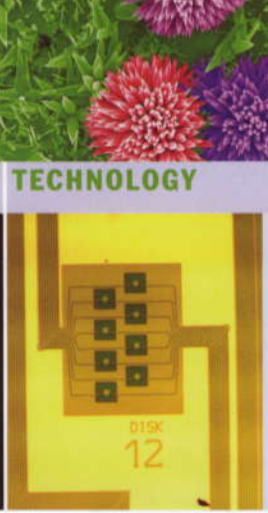

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Sophisticated models replicate the effects of tunnel junctions

LEDs, lasers and multi-junction solar cells can all employ tunnel junctions to improve performance. Calculating the effects of this junction is tricky, but there are ways to accurately simulate chip characteristics and cost-effectively optimize the structure's design, say **ZQ (Leo) Li** and **Simon Li**.

Leo Esaki's discovery of electron tunneling in p–n junctions in the late 1950s has left a legacy for our industry. Although major scientific recognition for his work came in the form of a shared Nobel Prize for Physics in 1973, an arguably even greater accolade has followed – the widespread use of the tunnel-junction structure based on his discovery in a wide variety of commercial devices.

Today tunnel junctions (see box "How a tunnel junction works", p30, for an explanation of the operating principle) appear in electronic and optoelectronic compound semiconductor devices to perform functions such as reducing resistance, preventing current crowding, linking devices together and providing electrical and optical confinement. In multi-junction solar cells they "glue" individual cells together and in LEDs they cut resistance and reduce current-crowding in p-type layers, leading to substantial increases in light extraction and uniformity. Tunnel junctions can also be used to stack bipolar cascade laser diodes together to form high-power bars that recycle electrons at each stage and produce an output proportional to the number of stages. In VCSELs, the junctions can provide electrical and optical confinement within the device.

It is important to cost-effectively optimize the design and processing methodology of the tunnel junction within each of these devices, which is possible with a technology computer-aided design (TCAD) approach. This has already been employed in the silicon industry for manufacturing CMOS chips, power devices and image sensors, but it is much more challenging to apply this technique to compound semiconductor optoelectronics.

For one thing, simulating optoelectronic devices is far more complicated. In addition to the Poisson equation (which calculates the electric-field gradients) and the carrier-transport equation that describe silicon devices, more equations are needed to calculate light generation (an optical-gain equation) and propagation (an optical-wave equation), alongside an approach that takes into account the coupling between these effects. Optoelectronic devices can also contain quantum wells and dot structures to confine the carriers, which means that the traditional drift-diffusion equation must be modified for these nanostructures. In addition, many of the material parameters for compound semiconductors that are needed for simulations are not well calibrated. Despite these immense challenges, the popularity of TCAD for the design of laser diodes, LEDs and photodetectors has grown in recent years.

At Crosslight, which is headquartered in Vancouver, Canada, we have developed a software package for modeling optoelectronic devices incorporating tunnel-junctions. We believe that this tool, which is called "advanced physical models of semiconductor devices" (APSYS), is the only piece of commercial software available for simulating this type of structure. Carrier transport of the tunnel-junction-based devices is modeled by drift-diffusion theory using a

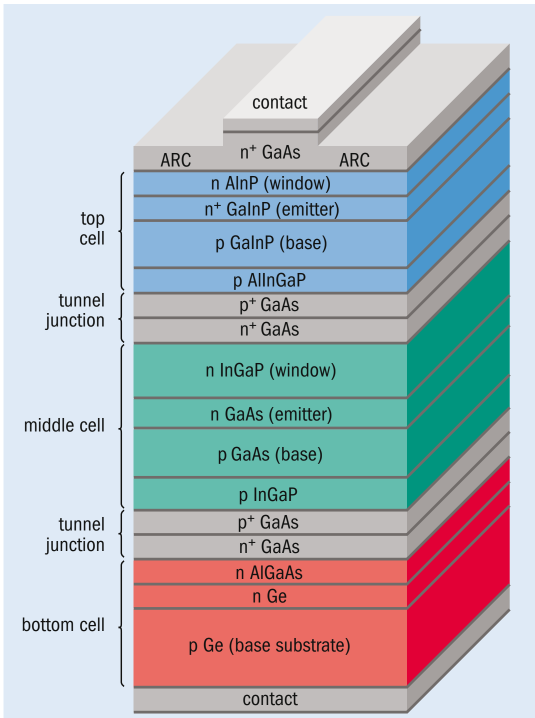
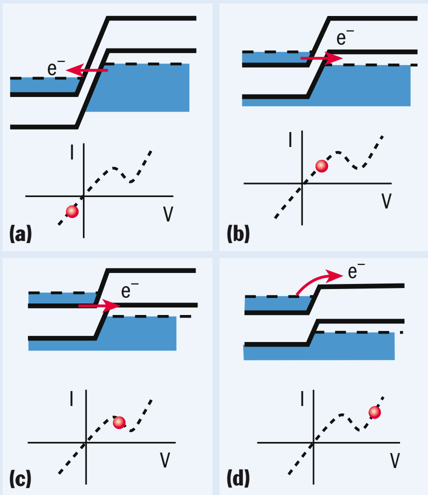


Fig. 1. Crosslight's software can model the band structure of devices containing tunnel junctions, such as triple-junction solar cells comprising sub-cells of germanium, GaAs and InGaP.

IBM

Leo Esaki discovered the tunneling effect that holds the key to tunnel-junction operation in 1957 when he was leading a small group of researchers studying the properties of germanium p–n junctions at Sony Corporation, Tokyo. Three years later he left Japan, joined IBM and started to pioneer the development of semiconductor quantum structures such as superlattices. In 1993 he retired from IBM and returned to Japan to become president of the University of Tsukuba.

What is a tunnel junction?



A tunnel junction is a heavily doped, thin p–n junction that has a negative resistance at certain forward bias values due to electrons tunneling from the n-side to the p-side.

The structure is formed from p-type and n-type layers with a typical thickness of 10 nm and a doping level of around $10^{20}\,cm^{-3}$. Heavy doping creates a "broken" bandgap, (denoted by the dotted lines in the figure), which leads to electron states in the conduction band on the n-side of the junction that are similar in energy to the valence-band-hole states on the p-side.

Under reverse bias (figure (a)) electrons tunnel in the opposite direction (from the p-side to the n-side). This results in different electron and hole states on each side of the junction that are increasingly aligned. Electrons can then tunnel through this junction from valence band to conduction band (a process called interband tunneling).

Under forward bias, voltage increases (see figure (b)) cause electrons to tunnel through the p–n junction due to the electron states on the n-side aligning with hole states on the p-side. When the voltage is further increased (figure (c)), these states become more misaligned and the current drops. This scenario is called negative resistance, because current decreases with increasing voltage.

As the voltage bias increases even further (figure (d)) the device begins to operate as a conventional diode. Electrons then travel by conduction across the junction, rather than tunneling through this barrier.

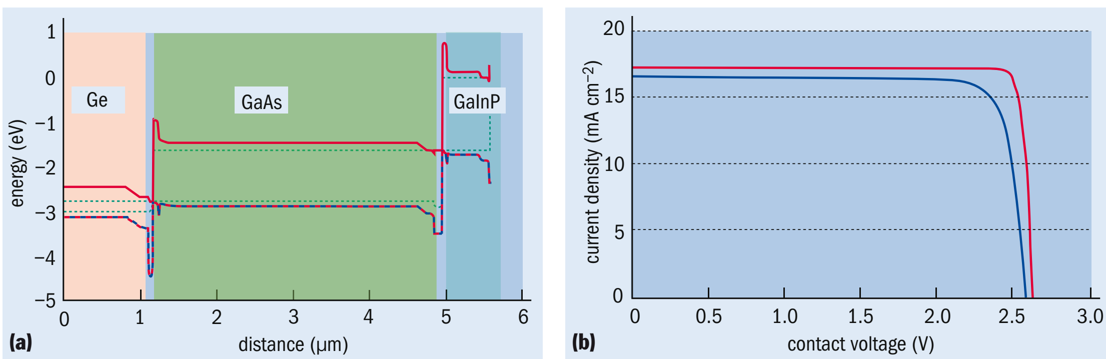


Fig. 2. (a) Crosslight's tool can calculate the band structure in a germanium, GaAs and InGaP solar cell under a bias of 3 V. The green dashed lines show the quasi-Fermi levels for the conduction and valence bands. The red line shows the conduction band throughout the structure. The dashed red and blue lines show the heavy-hole and light-hole valence bands. **(b)** Predictions of the short circuit current density for this triple-junction solar cell (red line) are in good agreement with the experimental results (blue line). The actual cell had a surface area of $21.65\,cm^{-2}$, a fill-factor of 85.15% and produced 0.783 W at an operating temperature of 28 °C and an efficiency of 26.7% under AM0 illumination.

finite-element approach. The electron density, hole density and electric potential at each mesh point form the basic variables; the other physical properties are calculated from these three quantities.

With a tunnel-junction structure, the current in the device depends on electron transport on one side of the junction and hole transport on the other. This means that the non-local nature of the inter-band tunneling current cannot be simply added into the drift-diffusion model, so a carrier generation term has been introduced into the layers to circumvent this issue. Tunneling is then modeled as another carrier generation mechanism, which depends on the local electric field and electron bandgap.

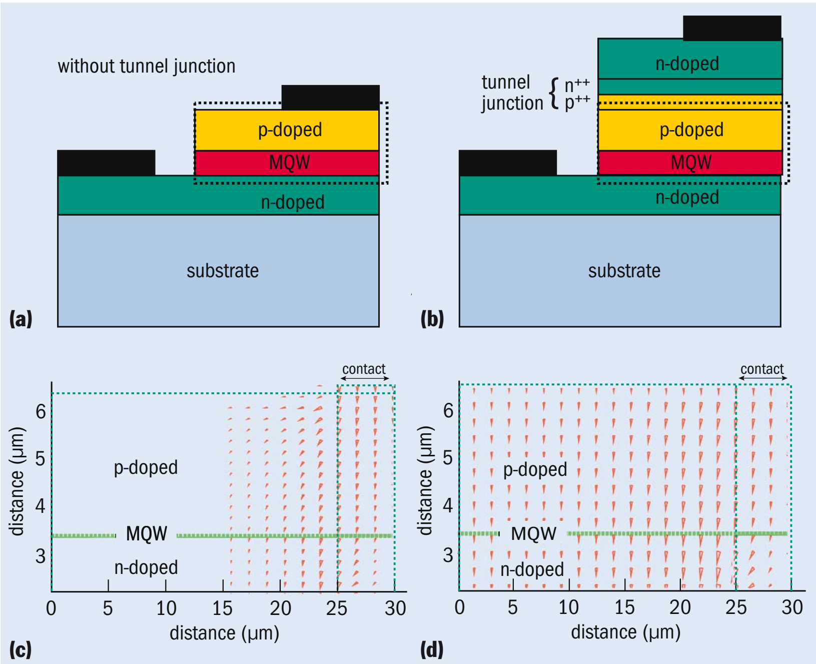
Our model shows that the tunnel junction's thickness is critical to device performance. If it is too thin it prevents depletion in the layer, but if it is thicker than strictly necessary it increases free-carrier optical absorption. Doping of the junction must also be sufficiently high to reduce electrical resistance, but not so high that it affects material quality. Compounding this delicate balancing act is the influence of the overall device structure on a particular optimization of the junction's thickness and doping level. This means that tunnel-junction optimization must be carried out in conjunction with all the other layers of the device.

Multi-junction solar cells

Our model can simulate the performance of multi-junction solar cells. It has been used to study a common structure that features three sub-cells: germanium, GaAs and InGaP junctions stacked in series (see figure 1, pX). The GaAs and InGaP sub-cells each have a bottom back surface field layer and a top window layer, and two tunnel junctions connect each pair of sub-cells. Solar-cell operation involves a complicated interaction between photons and electrons, the transport of carriers and the propagation of light through the tunnel junctions.

Our simulation has maximized this triple-junction cell's efficiency by optimizing every layer's thickness and doping density. This approach can calculate the positions of the valence and conduction bands throughout the entire structure (see figure 2(a)) and the device's current-voltage characteristics (see figure 2(b)). Predictions for short-circuit current, open-circuit voltage and efficiency are in very good agreement with experimental results.

Carrying out simulations is a cost-effective way to investigate the effects of new materials and different solar-cell structures on the efficiency of multi-junction structures. We have begun to study the performance of quadruple-junction solar cells employing an additional nitride layer. Initial results



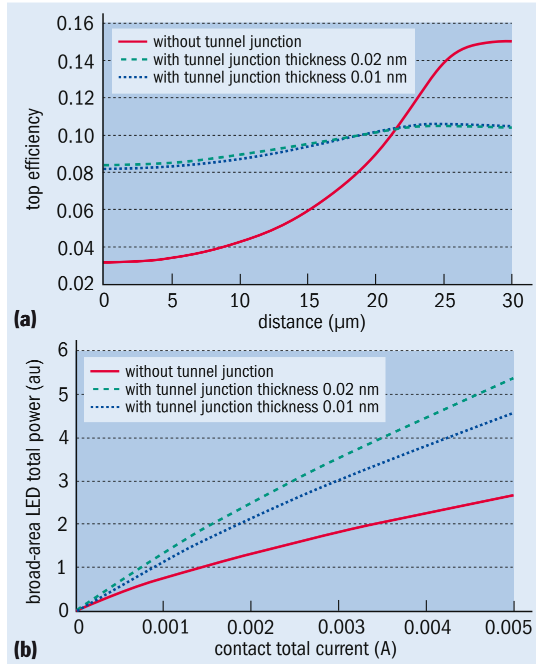


Fig. 3. (above) The addition of a tunnel junction to a conventional design (see **(a)** and **(b)**) improves current spreading beneath the contact and ultimately increases output power and emission uniformity. The vector plot **(c)** shows a current-flow simulation for the rectangular area outlined in **(a)**, which has a far less uniform current flow than that calculated for the tunnel-junction-based device **(d)**. **Fig. 4.** (right) Crosslight's simulations reveal the benefits of a tunnel junction on LED efficiency. The LED's "top efficiency", which is defined as the external efficiency across the top of the device, is much lower in the center of the conventional LED (distance = 0) due to current crowding. With a tunnel junction, the top efficiency and emission power (measured in arbitrary units) are substantially improved **(b)**.

suggest that this combination could boost overall conversion efficiencies to 43%.

Nitrides already feature in billions of blue and white LEDs. The commercial success of these chips is undeniable but their performance remains limited by poor current spreading, which results from a low hole concentration and high resistivity in the heavily doped p-type layers.

This problem can be overcome by either turning to a semi-transparent p-type electrode that improves current spreading and light extraction in top-emitting LEDs, or by switching the design to a flip-chip structure. However, both these approaches pay the penalty of more complex fabrication.

This pitfall can be avoided by adding a buried tunnel junction on the LED's p-side. It removes the need for lateral hole injection and can double the top-emitting power of blue LEDs, according to research from Seong-Ran Jeon and co-workers from Chonbuk National University, Korea. The US Air Force Research Laboratory (AFRL) has produced similar results with tunnel-junction structures that eliminate the hole-injection layer and provide a link between a stack of GaAs-based LEDs. The tunnel junctions improve the uniformity of the output power from this multi-LED emitter.

Typical LEDs employing a tunnel junction require three more epilayers than their conventional equivalents (see figure 3). With these additions, significant increases in output power are possible at the expense of only a small increase in operating voltage, if the thickness and doping profile of the tunnel junction has been optimized. Self-heating effects also need to be considered. To simulate all relevant effects in a coupled and self-consistent manner we have developed sophisticated models, which produce very good results.

Researchers William Siskaninetz and Thomas Nelson from AFRL have used our tool and commented: "The APSYS software by Crosslight gave us extremely accurate electrical predictions of our bipolar cascade LED structures as verified experimentally. We also received tremendous qualitative agreement in the light-output predictions."

The guidance provided by our simulations is illustrated in a comparison of LEDs with and without tunnel junctions. Calculations of the current flow reveal that the switch from a hole conduction layer to a tunnel junction dramatically improves current spreading beneath the p-contact (see figure 3). The greater current spreading also improves the uniformity of the LED's external emission (figure 4(a)), and the output power (figure 4(b)). All of these results are in very good agreement with experimental observations and demonstrate the benefits of accurate modeling for cost-effective device design and optimization.

Further reading

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S R Jeon *et al.* 2002 *IEEE J. Sel. Topics Quan. Elec.* **8** 739

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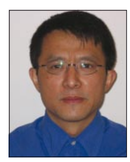


About the authors

Z Q Li (left) is vice president of engineering of Crosslight Software Inc. He has more than 50 research journal publications on modeling of semiconductor devices and materials, and previously worked for the National Research Council of Canada.

Simon Li (right) is president and chief software designer of Crosslight Software Inc. He has more than 20 years of experience in modeling semiconductor devices, and also worked for the NRC before founding the company.