Merging incompatible materials

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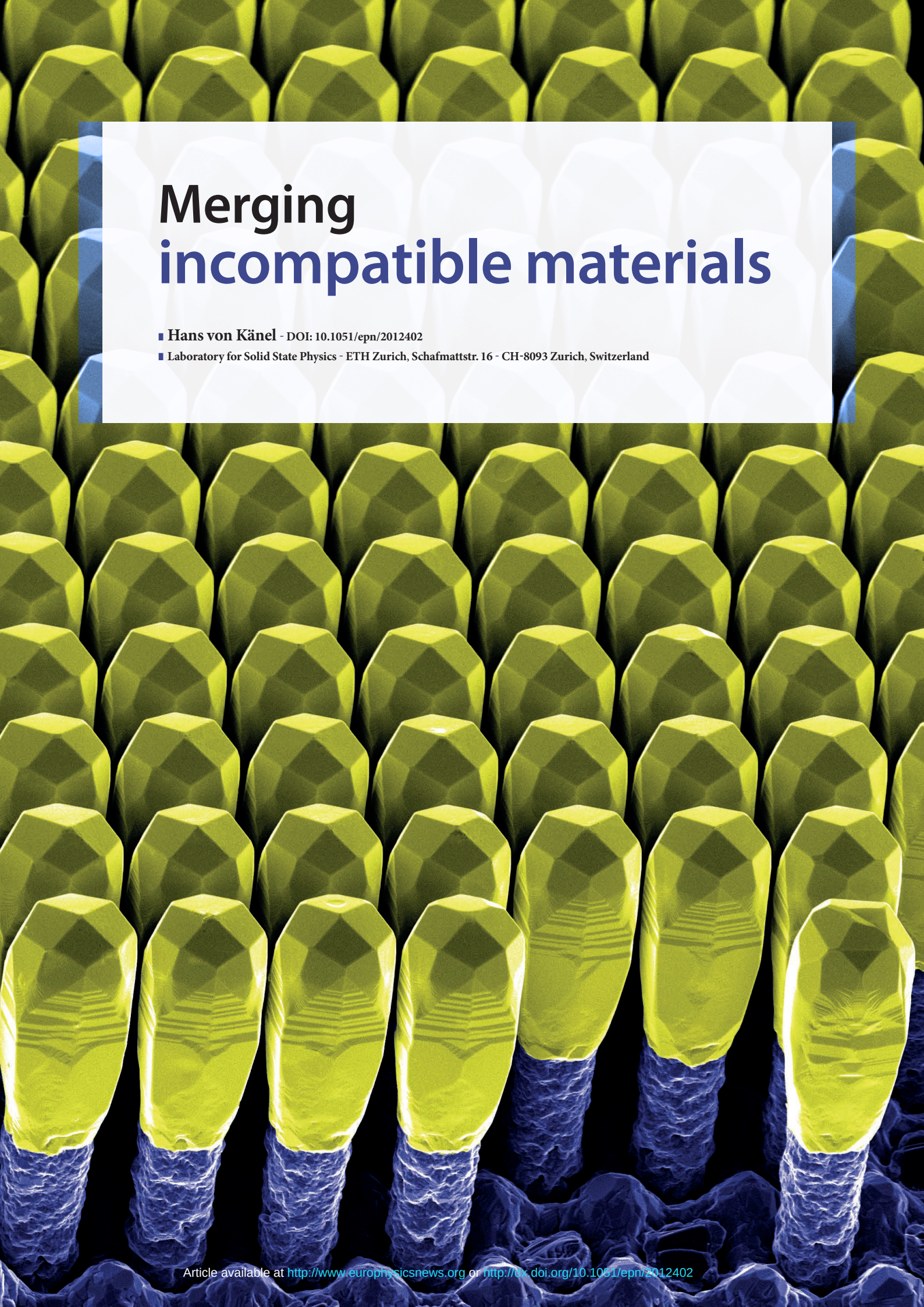


Highly perfect epitaxial semiconductor layers form the basis of many low-dimensional quantum structures and are used for ultrafast transistors, solid state lasers and detectors. Keeping epitaxial structures defect-free becomes difficult, however, when materials differ in lattice parameter and thermal properties. This often results in crystal defects, wafer bowing and cracks, unacceptable to any device application. These problems are solved by forming space-filling arrays of individual semiconductor crystals rather than continuous films.

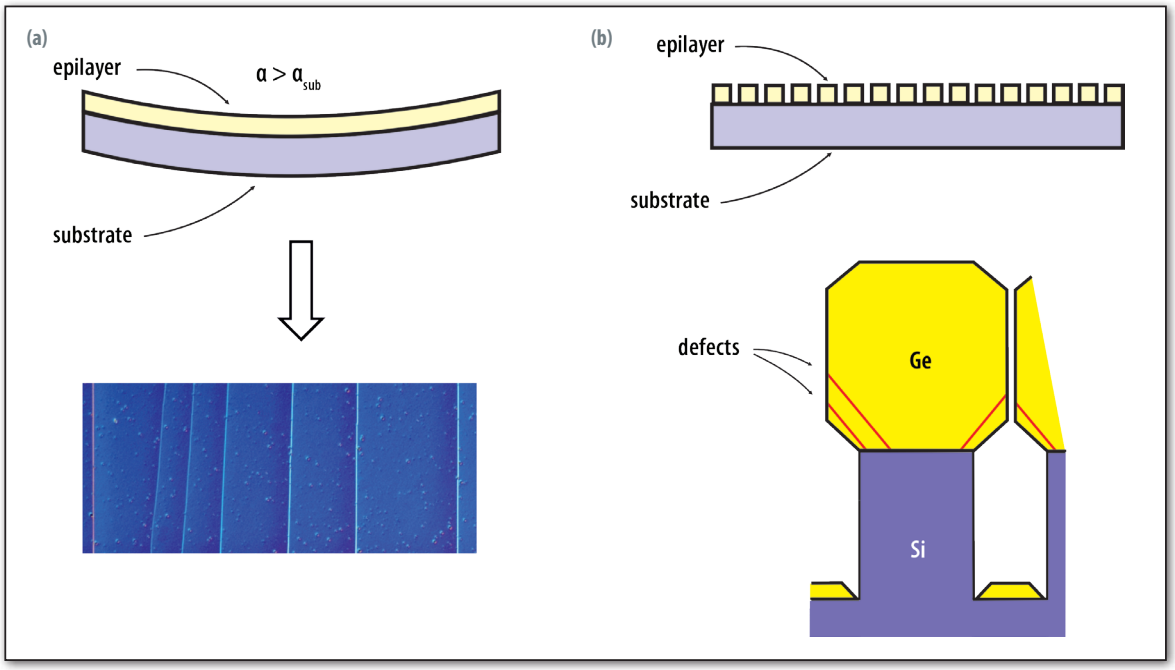
Ever since the pioneering invention of molecular beam epitaxy (MBE) in the late sixties by Arthur Cho [1], the tailoring of semiconductor properties by stacking different layers has been pivotal both for advances in fundamental research [2] and for the development of new semiconductor devices [3]. While much of the early work was focused on lattice-matched heterostructures, more and more use has been made lately of the additional degrees of freedom for band structure engineering offered by the misfit strain. Nowadays "strained-silicon" forms an integral part in most state-of-the-art microprocessors [4]. Many applications, such as high-brightness light-emitting diodes, power transistors, or multiple-junction solar cells, require rather thick epitaxial layers for which any misfit strain is totally relaxed at the growth temperature. Such layers may nevertheless become strained if their thermal expansion coefficients differ from the one of the substrate.

The role of lattice and thermal misfit

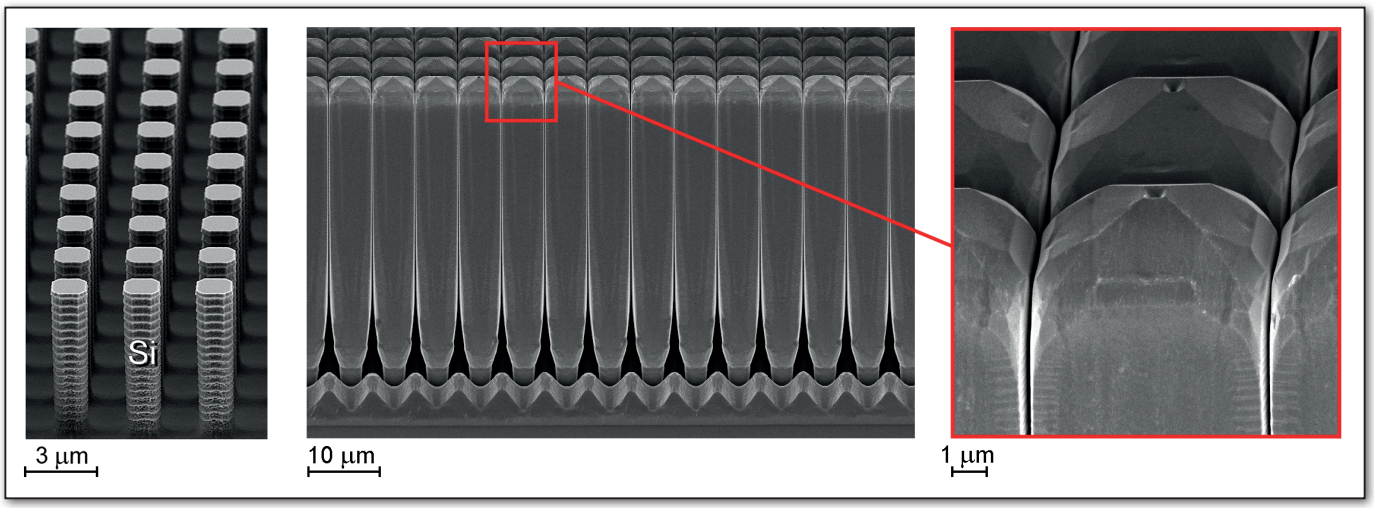
Irrespective of the technique by which an epitaxial layer is formed, complications arise whenever substrate and layer materials differ significantly in lattice parameter. According to theoretical studies originated by Frank and van der Merwe [5] the misfit across the interface is accommodated by misfit dislocations as soon as a critical thickness is reached. Unfortunately, in practice these dislocations are present not only at the interface. Misfit segments are rather terminated by threading dislocations extending throughout the epitaxial layer [6]. Since threading dislocations negatively impact performance whenever they penetrate an active region of a device, decades of intense work has sought to eliminate these defects or at least to minimize their density [7][8].

Since in addition to the lattice misfit, different semiconductors usually have different thermal expansion coefficients, wafers may bend upon cooling to room temperature. Very often layers even crack (Fig. 1(a)) when their thickness exceeds a few micrometers [9]. Wafer bending and layer cracking are hence of major concern, especially when multiple- junction solar cells, high-brightness light emitting diodes and power electronic devices are to be grown onto cheap Si substrates. Here, I shall discuss another extreme case, namely an X-ray absorber monolithically integrated on a Si-CMOS (Complementary Metal Oxide Semiconductor) chip [10]. Because of its higher atomic number germanium is considered to be a viable candidate for replacing Si as the absorbing material.

◂ Perspective-view scanning electron microscopy image of 8-µm-tall germanium crystals, epitaxially grown on a silicon wafer, patterned in the form of 8-µm-high and 2-µm-wide pillars, separated by 2-µm trenches.



◂ **FIG. 1:** (a) Wafer bending and crack formation because of thermal expansion coefficients of Si-substrate and Ge-layer differing by about 130%. (b) Concept for Si(001) substrate patterning and epitaxial growth to eliminate wafer bowing and cracks by avoiding a continuous film to form. Defects lying on {111} planes are expected to escape to the surface of the Ge crystals.



▲ FIG. 2: Si-pillars etched by deep reactive ion etching into Si(001) (left), subsequently overgrown with 50 µm of Ge (right). Note the finite gap between neighboring Ge crystals.

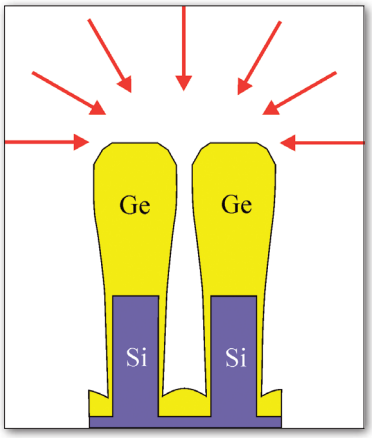
In contrast to compound semiconductors such as CdTe, it is compatible with Si processing. In order to efficiently absorb X-rays, a Ge layer must, however, be dozens of microns thick! How could one hope to grow such Ge layers crack-free and dislocation-free onto a Si substrate, which, moreover, is to remain flat, in view of thermal expansion coefficients differing by as much as 130%?

The main idea

Faced with the problem of fabricating an X-ray imaging detector monolithically integrated on a Si CMOS chip, we soon realized that the conventional means for thermal stress relief, such as very slow cooling or introducing stress-compensating interlayers, would never work. The only feasible way appears to be replacing a continuous layer by a dense array of individual crystal blocks [10]. *But this has to happen spontaneously during crystal growth, since after cooling down it would be too late, as by then the layer would already have cracked!*

The basic idea is outlined in Fig. 1(b). In a first step the Si substrate is patterned by photolithography and deep reactive ion etching, preferably in the form of tall pillars a few microns in width, separated by several µm wide trenches. What happens now when Ge is epitaxially grown onto such a patterned Si surface? Clearly, any growth carried out close to equilibrium would tend to flatten the surface and inevitably lead to a continuous film. Growth must therefore proceed far from equilibrium in a kinetic regime.

▼ FIG. 3: Shielding of particle flux arriving at the surface of closely spaced Ge crystals.



Loosely speaking, this means using high deposition rates and low substrate temperatures. Our method of choice has been low-energy plasma-enhanced chemical vapor deposition (LEPECVD) [11], a method permitting growth rates of several nm/s, far above the ones of thermal CVD at substrate temperatures around 500° C. Under such conditions Ge atoms diffuse short distances before being incorporated into the growing crystal, typically on the order of 100 nm.

Space-filling epitaxial crystal arrays

The combination of deep substrate patterning and epitaxial growth far from equilibrium does indeed produce the desired result to a surprising extent. According to Fig. 2, the Ge crystals nucleating on the top of the Si pillars at first exhibit both vertical and lateral growth. Their lateral expansion comes to a complete standstill, however, once the Ge crystals reach a certain height, depending on the spacing of the Si pillars. The final gap amounts to about 50 nm and seems to persist to virtually arbitrary height as exemplified by the 50 µm tall crystals. High-resolution X-ray diffraction measurements show that the thermal strain of the Ge crystals is completely relaxed as opposed to the unpatterned parts on the same substrate where the cracked Ge layer is under a residual, thermally induced, tensile strain. Inclined surface facets are known to deflect threading dislocations towards the sidewalls of growing crystals [12]. We have indeed found no evidence for dislocations at the top of fully faceted Ge crystals, neither by high-resolution transmission electron microscopy nor by chemical etching and etch pit counting.

The mechanism for the unusual mode of epitaxial growth, leading to the space-filling crystal arrays of Fig. 2, has been studied by theoretical modeling [10]. The main ingredients of the model are a negligibly small surface diffusion length and mutual flux shielding by neighboring crystals. This can be understood from the scheme of Fig. 3, depicting the flux of activated species incident on the growing crystals. This flux is composed of a vertical and an isotropic component. The closer the crystals approach each other as growth proceeds, the more the sidewalls are shielded from the isotropic component and the more their lateral expansion is reduced.

Concept of an X-ray imaging detector

How can the Ge crystal arrays of Fig. 2 be used in an X-ray imaging detector? Our concept of such a detector is schematically depicted in Fig. 4. Here, the absorber layer is made from lightly p-doped Ge crystals grown onto the backside of a thinned, lightly n-doped Si wafer.

The readout CMOS circuits will be fabricated on the front side of the wafer in implanted p-wells. The p-doped Ge crystals and the n-doped substrate together form heterojunction p-n diodes, which, under a reverse bias voltage, permit the separation of electron-hole pairs generated by X-ray photons absorbed in the Ge. The Ge crystals are mutually isolated electrically by an oxide coating on the Si pillars. The heterojunction diodes can thus be characterized individually inside a scanning electron microscope. Ohmic contacts to the Ge crystals are formed by focused ion beam deposition of platinum. An example of a current-voltage curve, obtained by contacting a Ge crystal by a tungsten tip, can be seen in Fig. 4. The reverse current of the order of 1 mA/cm^2 at -15 V is comparable to commercial Ge p-i-n diodes of much larger size.

Diffraction measurements show that the thermal strain of the Ge crystals is completely relaxed

In principle, individual contacting of Ge crystals a few microns in width may be imagined to give rise to an imaging detector with enormous spatial resolution. In practice, however, X-ray photons impinging at an oblique angle are expected to be absorbed by several crystals. This, together with the finite thickness of the Si substrate, will degrade the spatial resolution. For this reason the pixel size of the actual detector is defined by the spacing of the n$^+$ implants rather than the size of the Ge crystals. This has the advantage that only one single metal contact is required on the absorber side.

What next

A high-resolution X-ray imaging detector based on epitaxial Ge crystals monolithically integrated on a CMOS chip is but one of the applications enabled by the new mode of substrate patterning and epitaxial growth. The extension of the concept to other material combinations is currently under way in the areas of high-efficiency solar cells and power electronic devices. ■

About the author

Hans von Känel is a lecturer at the ETH in Zurich and former full professor of physics at the Politecnico di Milano. His fields of interests comprise phase transitions, interfaces and surfaces, scanning probe techniques, and epitaxial growth. Besides his activities in the academic world he has been involved in technology transfer and the founding of start-up companies.

Acknowledgment

The author is grateful to his colleagues C.V. Falub, A. Gonzalez, T. Kreiliger and E. Müller from the ETH; to A. Dommann, R. Kaufmann, A. Neels, P. Niedermann, and A. Pezous from the CSEM; G. Isella, D. Chrastina, S. Cecchi and F. Isa from the Politecnico di Milano; L. Miglio, R. Bergamaschini, and A. Marzegalli from the Università di Milano Bicocca. Financial support by the Swiss Federal Program Nano-Tera through the projects NEXRAY and COSMICMOS is gratefully acknowledged, as well as partial support from Fondazione Cariplo within the MANDIS project.

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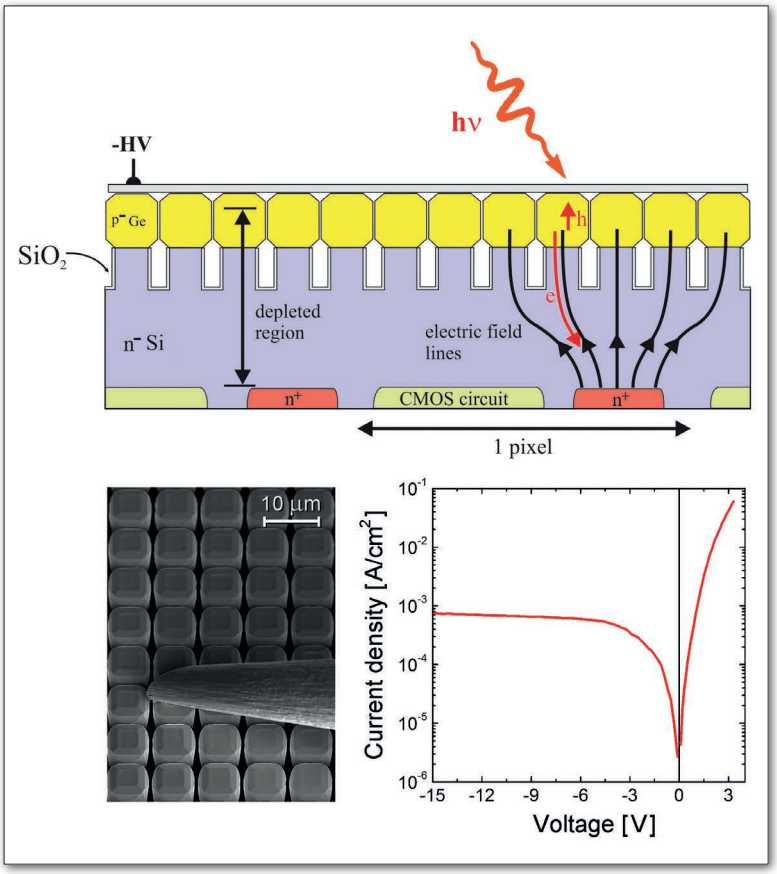

▼ **FIG. 4:** Concept of an X-ray imaging detector with a monolithically integrated Ge-absorber on a CMOS chip and current-voltage curve of a single Ge/Si(001) heterojunction measured inside a scanning electron microscope.