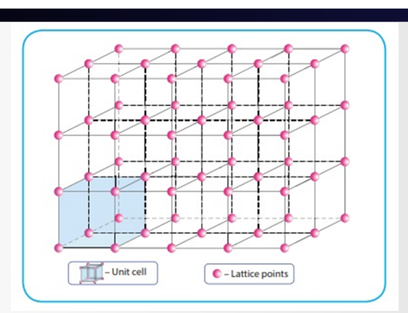
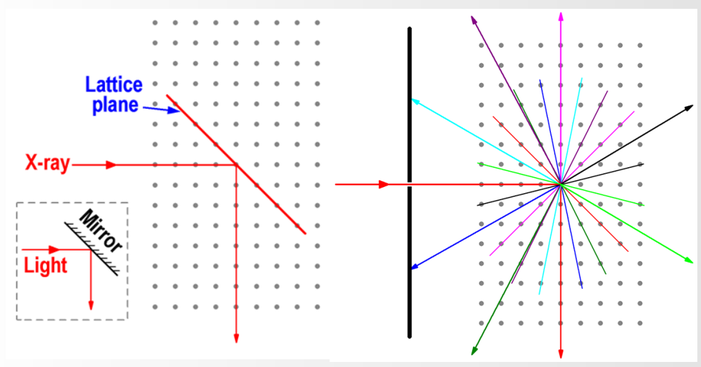
# A Smart Computer Program LauePt4 for Recognizing and Simulating Laue Patterns and Its Applications

## INTRODUCTION




Lattice structure of a crystal. Image from byjus.com

- A crystal is a solid material with the constituent atoms, molecules, or ions periodically arranged to form a lattice
- The unit cell is the smallest unit of volume that is repeated over and over in all directions so that the entire periodic crystal lattice is constructed.

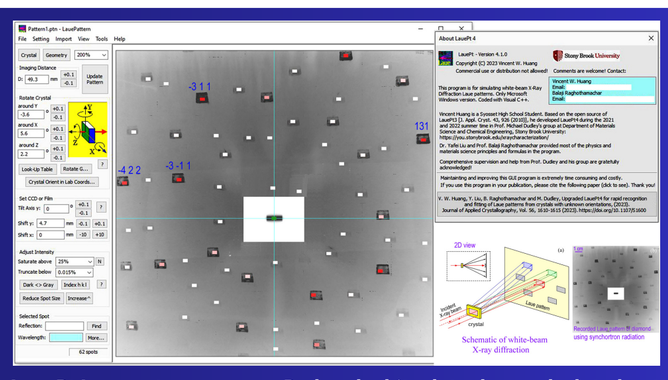



X-ray diffraction by a single (set of parallel) lattice plane(s) similar to mirror reflection. The periodic dots represent lattice points of the crystal. Figure created by student researcher

- X-rays are extremely short-wavelength light.
- X-rays can be reflected by Lattice planes inside a crystal (not the surface), called X-ray diffraction.
- The geometry of X-ray diffraction is the same as visible light reflection if we consider the lattice plane as a mirror! (The incidence angle is always equal to the reflection angle)
- However, Laue patterns cannot be reliably interpreted by eye, an enduring problem in crystallography

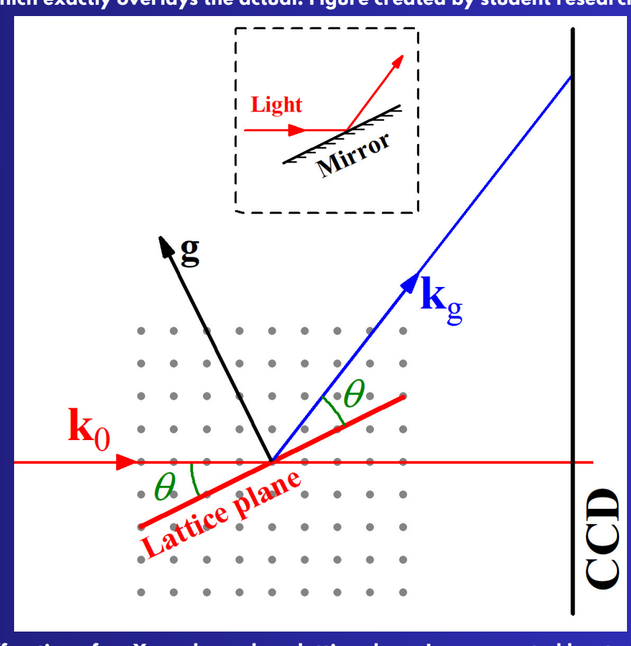
## *LAUEPT4* COMPUTER APP

- A full-function computer application written in Visual C++ and Microsoft Foundation Classes
- Small single-size executable file (2.5MB)that can run on any Windows computer
- User-friendly graphical interfaces can be readily used by non-specialists without training without crystallography knowledge
- Capable of simulating,recognizing, and analyzing Laue patterns of any crystals with arbitrary orientations.



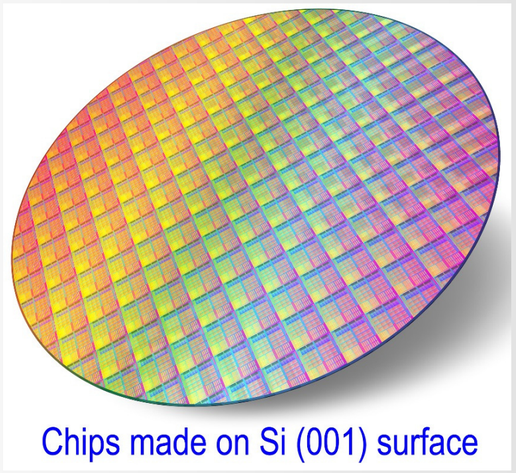

The LauePt4 computer program. Red and white dots show calculated pattern, which exactly overlays the actual. Figure created by student researcher

- A crystal structure can be described by three primitive vectors a, b, c, three angles alpha, betta, gamma
- A lattice plane can be identified by three Miller indices (h,k,l)
- The normal to th e lattice plane can be calculated witih geometry
- LauePt4 calculates Kg and every point on the Laue pattern
- Three novel methods allow quick identification of arbitrary patterns as well




Diffraction of an X-ray beam by a lattice plane. Image created by student researcher.

## APPLICATIONS




(Image from https://nanografi.com/blog/explained-silicon-wafers-and- its-applications/)

- LauePt4 can determine exact crystal orientation, which is critical for semiconductor manufacturing
- Chips must be exactly cut along their specific internal orientations.
- LauePt4 can also be used for white-beam X-ray topography characterization of crystals, critical in research of next-generation semiconductors such as silicon carbide
- Such semiconductors are used in electric vehicles, 5G cellular networks, and cutting-edge AESA radars
- LauePt4 is already in professional use at a number of national laboratories and universities

## SELECTED REFERENCES

The main results of this work has been published in Huang, V. W., Liu, Y., Raghothamachar, B., & Dudley, M. (2023). Upgraded LauePt4 for rapid recognition and fitting of Laue patterns from crystals with unknown orientations. Journal of Applied Crystallography, 56(5), 1610–1615. (and see references therein).