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CrystalWalk: crystal structures, step by step

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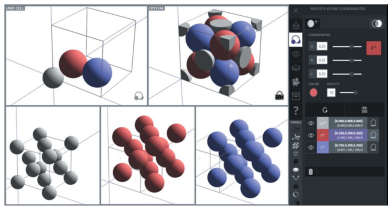
CrystalWalk is a crystal editor and visualization software designed for teaching materials science and engineering. Based on WebGL/HTML5, it provides an accessible and interactive platform to students and teachers by introducing a simplified crystallographic approach that creates crystal structures by combining a lattice with a motif without the use of its internal symmetry. *CrystalWalk* is the first software to use solely translational symmetry, aiming to introduce engineering students to the basic concepts of lattice and motif. Although very restrictive from the crystallographic point of view, *CrystalWalk* makes it simple for students to experiment, reproduce and visualize, in an interactive manner, most of the crystal structures that are commonly introduced in materials science and engineering curricula.

1. Introduction

CrystalWalk is a crystal editor and visualization software designed for teaching materials science and engineering. Based on WebGL/HTML5, it provides an accessible and interactive platform to students and teachers by introducing a simplified crystallographic approach that creates crystal structures by combining a lattice with a motif without the use of its internal symmetry. Avoiding the concept of space groups and internal symmetry is a didactic strategy often used in engineering textbooks (Van Vlack, 1989; Askeland, 1990; Smith, 1995; Callister & Rethwisch, 2007), and although elementary from the crystallographic perspective, *CrystalWalk* is the first software to effectively implement this approach. After choosing a crystal's lattice and entering the atomic coordinates of the translational or complete motif – as described by, for example, Tilley (2006), DeGraef & McHenry (2007) and Hammond (2009) – unit cells are automatically generated through the rigid sphere model and the lattice and atomic radii data incorporated into the software. Despite being very restrictive from the crystallographic point of view, using solely translational symmetry provides a useful tool to introduce engineering students to the basic concepts of lattice and motif. *CrystalWalk* makes it simple to experiment, reproduce and visualize, in an interactive manner, most of the crystal structures that are commonly introduced in materials science and engineering curricula.

Fig. 1 illustrates the example of the calcium fluoride (CaF_2) structure, popularly known as fluorite, a crystal structure where the fluorine sublattice is commonly misunderstood as a simple cubic lattice by students who may lack the skills to properly identify the neighbourhood of the fluorine ion in the representations of most textbooks (Fig. 1*a* and 1*b*). The use of *CrystalWalk* makes it simple to explore and visualize its three-ion motif (one Ca and two F) and its relationship with the face-centred cubic lattice and sublattices independently for



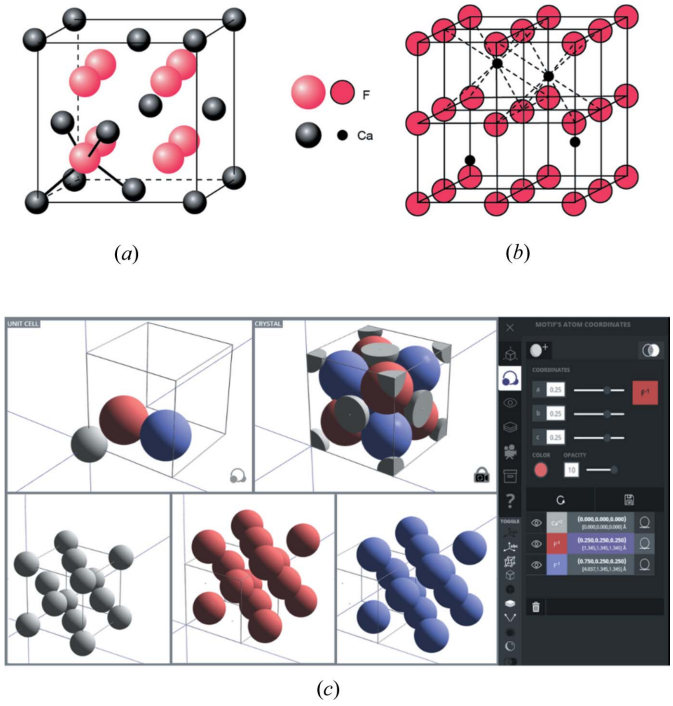


Figure 1
Unit cell of CaF_2 with (*a*) Ca atoms positioned externally, at the faces and edges of the cell, and (*b*) Ca atoms positioned internally. (*c*) *CrystalWalk* interface (adapted) displaying the fluorite motif, with the cropped unit cell and sublattices of Ca (grey) and F (red and blue). Source: (*a*) adapted from Askeland (1990); (*b*) adapted from Callister & Rethwisch (2007).

each member of the motif. This relationship can be easily observed in Fig. 1(*c*), where each member of the motif has been individually coloured. It is important to highlight *CrystalWalk*'s unique translational symmetry approach, which requires three atoms to define the fluorite motif, while existing crystallographic software uses the minimal asymmetric unit with only two atoms (one Ca and one F).

By consulting powder diffraction files and crystallographic tables it is still possible to use *CrystalWalk* to create more complex structures by entering individual coordinates from the translational motif. Although this would be laborious and very time consuming for fundamental crystallographic use, exposing students to this task does have its didactic value. *CrystalWalk* has a step-by-step tutorial that guides more adventurous users through this process.

Additionally, a comprehensive set of didactic functionalities is available, as an online content publication platform for sharing interactive crystal structures, a 'didactic narratives' tool that enables users to generate interactive classes based on predefined animated sequences as well as providing support for advanced interaction and virtual reality technologies such as Oculus Rift, Google Cardboard, LEAP Motion, multi-touch devices and three-dimensional printing technologies.

The development of *CrystalWalk* was guided by the free software philosophy, adopting state-of-the-art technologies for interactive web applications. *CrystalWalk* can be accessed online at http://cw.gl from desktop, mobile and tablet devices and its source code is openly available at https://github.com/gvcm/CWAPP.

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