



Porting Crystal Structure Data to Virtual Reality Using CAD2VR

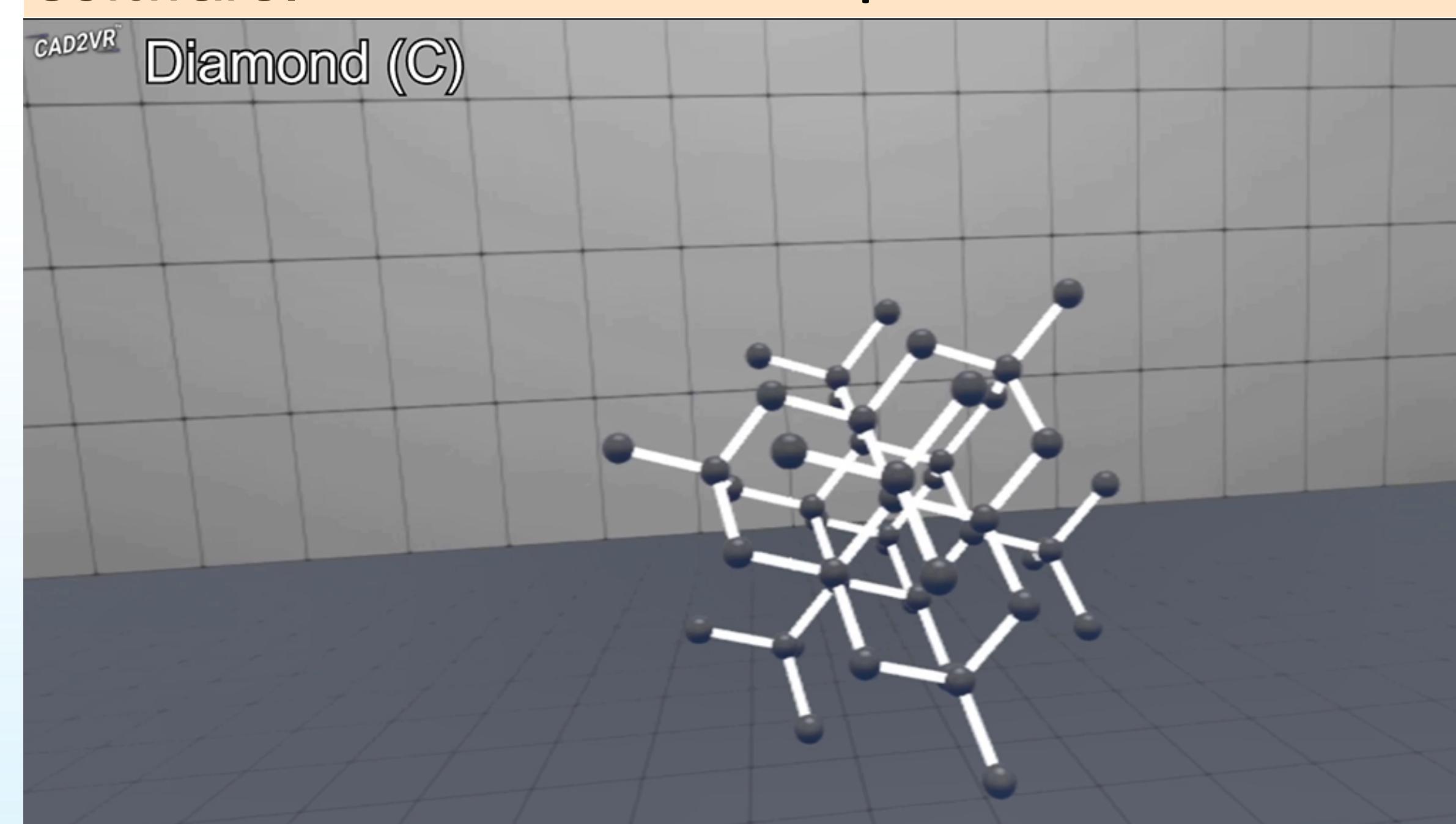
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Introduction

Computer-Aided Design (CAD) models are used in a variety of design applications, including engineering, architecture, product design, and manufacturing. CAD models can render 3D objects, but are typically limited to 2D displays.

CAD2VR was created at Sandia National Laboratories with the purpose of allowing users to interact intuitively with any CAD model in Virtual Reality (VR). The user can manipulate the model with a VR headset and handheld controllers, or with a keyboard and mouse in desktop mode. The software features both disassemble and reassemble modes as well as X-ray vision to see inside assembled or individual components. Other features include teleporting for use in small spaces, video camera placement, and interaction with a tablet that can mirror a display from the computer running the software.

Structure Manipulation



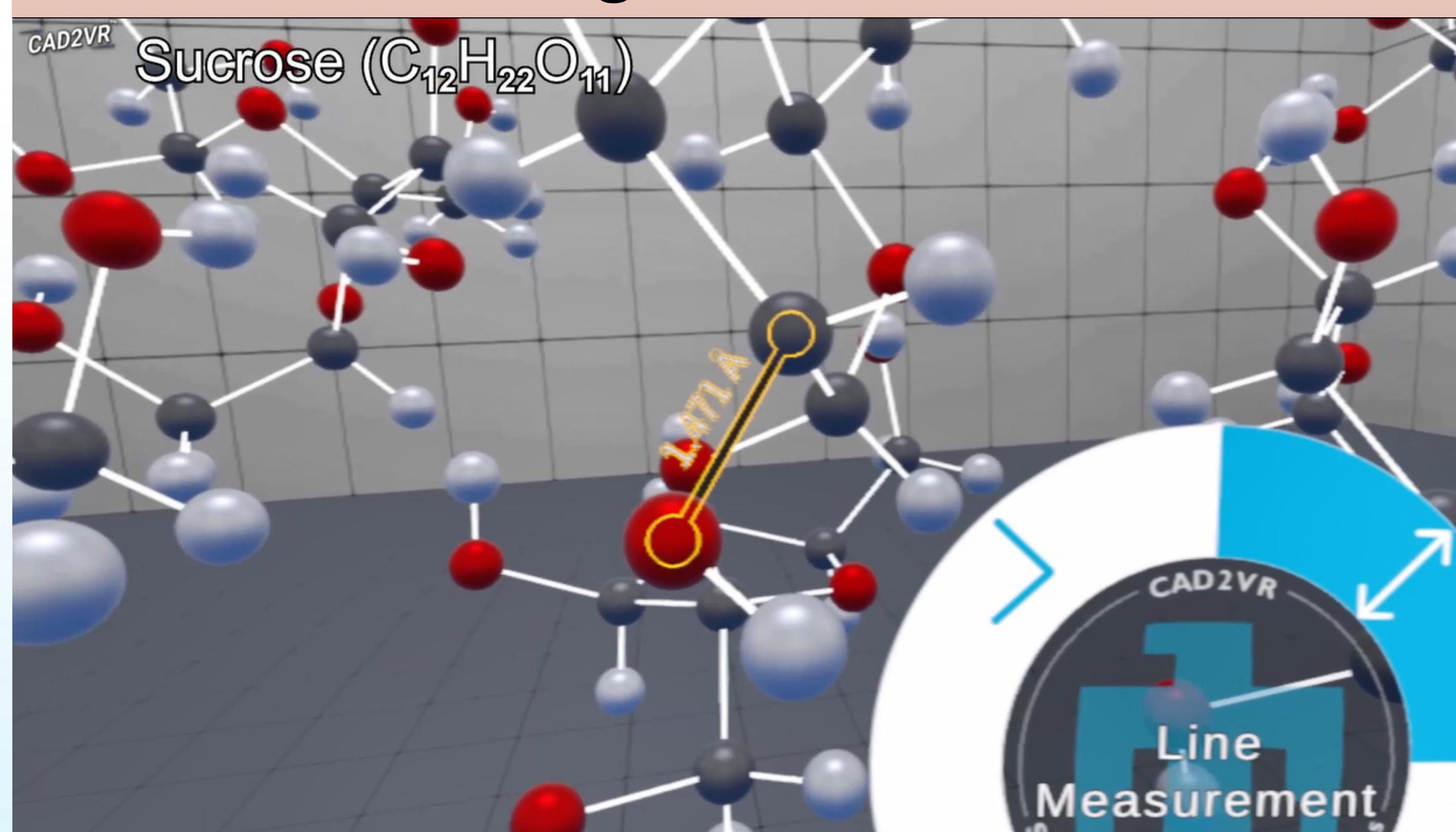
Integration to CAD2VR

The core CAD2VR software is designed to be adaptable to lab-wide applications through the use of plug-ins. Early attempts to display crystal structure data in CAD2VR were successful only in importing a rigid ball-and-stick molecule, similar to what can be fabricated with a 3D printer.

New capabilities allow the import of discrete atoms and the automatic drawing of bonds using adjustable tolerances. A new measurement tool was developed in parallel to the crystal structure import process and allows an existing measurement tool to latch onto the middle of a spherical shape. This is ideal for measuring the bond length or bond angle between atoms.

The images below display some of these features.

Bond Length Measurement



Future Work

The crystal structure viewing plugin is still at the prototype stage, and certain features are currently unrealized. CAD2VR cannot currently read a .CIF, which contains valuable information needed to render anisotropic atoms and grow the structure.

A working beta would ideally import data from the .CIF to aid the structure refinement process by displaying Q-peaks and atomic positions. The visual data from the .CIF could then be combined with the tablet feature of CAD2VR to display structure refinement files such as the .RES or .INS.

Other desirable features include drawing polyhedron volumes to measure void spaces and toggling the display of the unit cell.

Bond Angle Measurement

