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DWBuilder: A code to generate ferroelectric/ferroelastic domain walls and multi-material atomic interface structures

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Summary

In ferroelectric materials, the order parameter polarization can be switched by an external electric field. Regions within ferroelectric materials with uniform polarization are called domains, and the boundaries between domains with differently aligned polarization vectors are called domain walls (DWs). These domain walls, which are only a few nanometers wide, possess unique properties with potential technological applications. DWs show promise for nanoscale electronic circuit elements and enable innovative design concepts because they can be created, erased and moved using applied electric fields (Bednyakov et al., 2018; Catalan et al., 2012; Meier, 2015; Meier & Selbach, 2022). DWs can also replicate the functionality of key electronic components such as diodes (Whyte & Gregg, 2015), transistors (Mundy et al., 2017), and random access memories (RAM) (Sharma et al., 2017).

Due to the nanoscale sizes and promising properties of DWs, there has been significant interest in studying how to control and manipulate them using atomistic simulations (Schultheiß et al., 2020; Didrik R. Småbråten et al., 2018; Didrik Rene Småbråten et al., 2020). However, developing atomic DW structures is challenging and requires knowledge of the order parameter and DW types in ferroelectric materials. DWs can be ferroelectric, antiferroelectric, and/or ferroelastic, and they can vary depending on the allowed symmetry of the ferroelectric material. For instance, ferroelectric $BiFeO_3$ exists at room temperature as a rhombohedrally distorted perovskite with space group R3c and spontaneous polarization oriented along the $[111]_P$ axis (Ederer & Spaldin, 2005; Wang et al., 2003). The symmetry constraints of having the ferroelectric polarization in $BiFeO_3$ along <111> directions gives four types of DWs across which the polarization direction changes by 71°, 109°, or 180° (Wang et al., 2003). Similarly, other domain wall types have been identified in other ferroelectric materials such as $BaTiO_3$ (Taherinejad et al., 2012), $PbTiO_3$ (Meyer & Vanderbilt, 2002) and $YMnO_3$ (Didrik R. Småbråten et al., 2018), and in ferroelastics like $CaTiO_3$ (Barone et al., 2014).

The `DWBuilder` code is designed as a command-line tool to create DWs and interface structures from specific input unit cell geometries, as described in detail in the README file of the repository. The code comprises two main components: (i) a domain wall builder for similar materials and (ii) a heterogeneous interface builder for multi-material atomic interfaces. Figure 1 explains the structure and workflow of the `DWBuilder` package.

The first part, handled by the scripts `dwbuilder.py` and `dbuilder.py`, produces domain walls by first analyzing the input unit cell geometry and determining the space group of the structure. The space group is identified using the open-source Python library Pymatgen. If the space group matches the specified type, the script offers a range of possible domain wall types and ultimately creates the DW structures. If the space group of the input structure does not match, the script allows you to choose a desired space group type or manually define the domains by

specifying lattice vectors. To generate different domains separately, you can use `dbuilder.py` to develop distinct domains, which can be useful for bulk and surface calculations.

The second part of the code involves creating a heterogeneous interface structure of multi-material compounds, which is handled by the script `hibuilder.py`. This script requires two input structures, named `bulk1` and `bulk2`. To develop compatible interfaces, you must define the orientation relationship (OR) between the two bulk phases. This definition is necessary to address any lattice and angular mismatches that arise from differences in space groups and/or atomic structures of the two phases.

Currently, the script cannot predict the ORs that would result in a low lattice mismatch between the two bulk phases. However, theoretical studies and methods such as edge-to-edge (Zhang & Kelly, 2005) and face-to-face (Khalid, 2020) matching techniques can help predict low lattice misfit for interface construction. This script assumes that the user is already familiar with the appropriate ORs to construct the interface structure. For instance, the ORs of interfaces reported in referenced papers (Khalid et al., 2019, 2020, 2021; Khalid, Friis, Ninive, Marthinsen, Ringdalen, et al., 2021) can be replicated using this script. Additionally, the script can generate atomic interfaces if you know the OR from experiments, and it can predict the atomic interface structure and lattice mismatch between the two bulk phases.

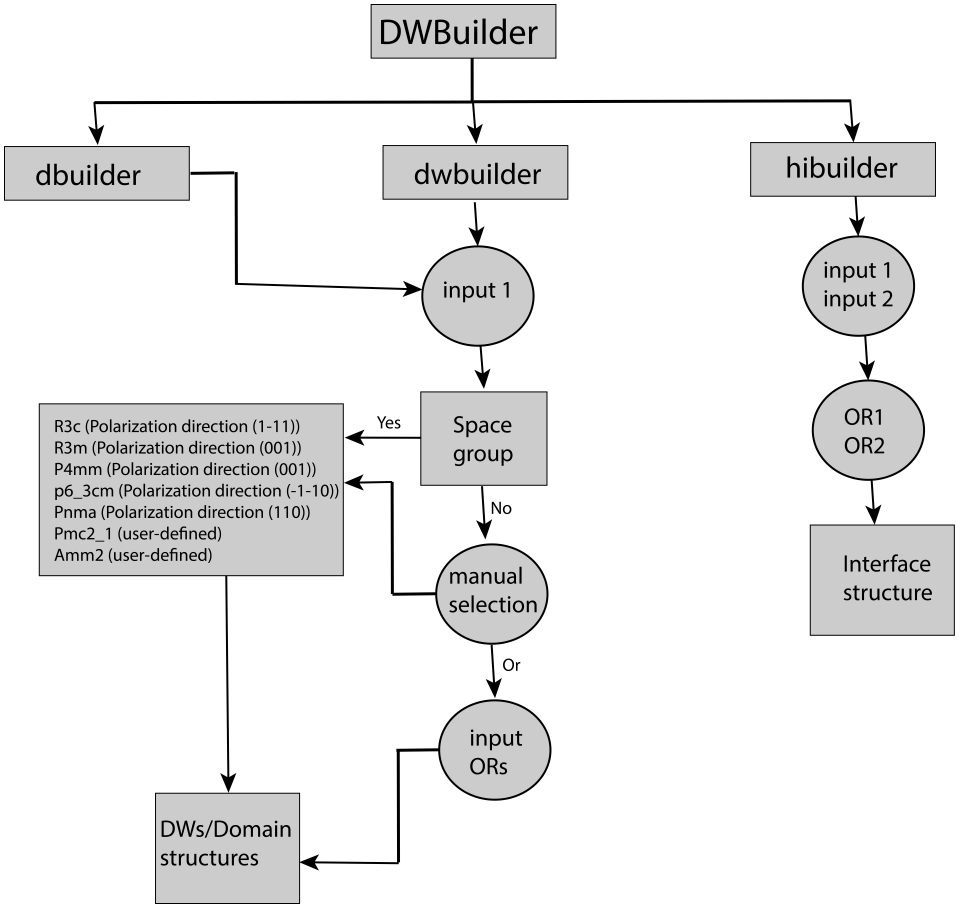

Figure 1: Structure of the `DWBuilder` package.

Statement of need:

`DWBuilder` is an interactive toolbox for developing atomic-scale domain walls and interface structures of homogeneous and heterogeneous material compounds, making it suitable for

high-throughput calculations. Its target audience includes students and scientists in materials science and physics at any level of expertise. `DWBuilder` utilizes the NumPy library extensively, which speeds up execution, particularly when working with large structures. Users are guided through the process of identifying and creating the desired domain walls in a step-by-step manner. The code is designed to be user-friendly and educational, with a focus on plane orientation and electric polarization switching.

The `DWBuilder` code is designed to automate the creation of atomic interfaces and domain wall structures, allowing researchers to focus on optimizing and studying material behavior and properties. The structures generated by this code are compatible with both first-principles and second-principles calculations. The code provides ample functionality to support practical research tasks while remaining lightweight and well-documented. This allows junior researchers with minimal or no assistance to easily install, use, and understand the code.

Example 1:

The below example demonstrates the functionality and steps of the `dwbuilder.py` script. Running the `dwbuilder` script will perform the following steps:

1. **User Input**:
   - Specify the script to run on the input structure.
   - Input the VASP format structure.
2. **Space Group Determination**:
   - The script determines the space group of the provided structure.
3. **Allowed Domain Wall Types**:
   - Based on the determined space group, the script identifies the allowed domain wall types.
4. **Domain Wall and Supercell Size**:
   - User inputs the desired domain wall size.
   - User specifies the supercell size for the domain wall structures.
5. **Final Domain Wall Structures**:
   - The script generates the final domain wall structures.
   - It prints any lattice misfit information.

Figure 2 illustrates an example of P4mm $PbTiO_3$ and hexagonal manganite $YMnO_3$ domain wall structures.

For proper ferroelectrics, such as perovskites ($PbTiO_3$, $BaTiO_3$, $KNbO_3$, etc.), the user only needs to define the primitive unit cell structure. The `DWBuilder` automatically determines the space group and constructs the respective domains and domain wall structures.

In certain cases, if the space group of the input structure does not match the defined space group type of the domain walls, the user can manually build the domains. This can be done by defining the transformation matrix of each domain using either `hibuilder.py` or by selecting the manual option for domain selection in `dwbuilder.py`.

For hexagonal manganites, both domain structures are required to build domain wall structures, as illustrated in Figure 2.

Example 2:

The following example illustrates the use of the `hibuilder.py` script. This script performs the following steps:

1. Inputs the primitive unit cell structures of the domain or bulk structures,
2. Defines the compatible transformation matrices for both input domains or bulk structures,
3. Develops the transformed bulk structures,

4. Stacks the transformed bulk structures to build the final interface and calculates the lattice and angular misfit.

Figure 3 illustrates an example of the interface structure between Fe and Fe_2Al_5. This example is taken from the study by (Khalid, Friis, Ninive, Marthinsen, Ringdalen, et al., 2021).

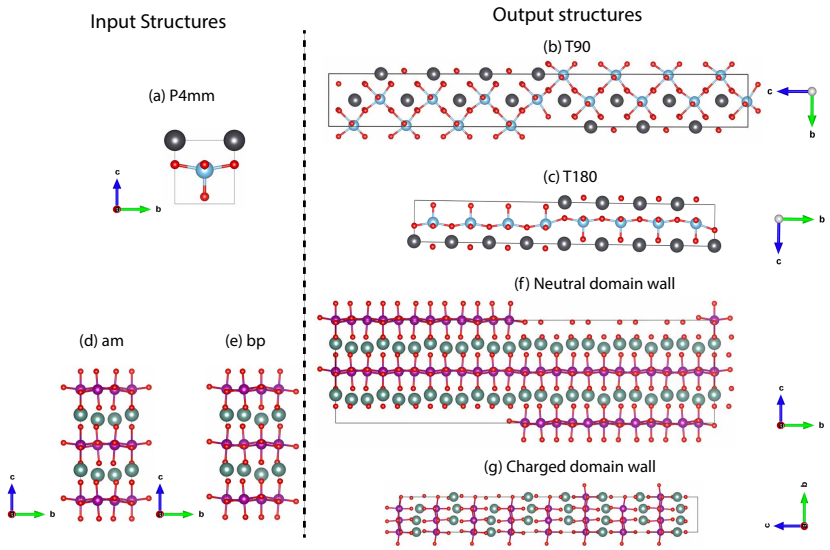

Figure 2: Illustration of domain wall structures in $PbTiO_3$ and $YMnO_3$ using the `dwbuilder.py` script. $PbTiO_3$, a proper ferroelectric belonging to the tetragonal P4mm space group, exhibits a polar axis along the c-axis in the primitive unit cell structure, as shown in (a). The `DWBuilder` script automatically determines the space group and constructs the (b) T90 and (c) T180 domain wall structures. For $YMnO_3$, with two domain structures, (d) am and (e) bp, both exhibiting polarization along the $\pm c$-axis, the script generates (f) neutral domain walls by stacking the domains along the b-axis and (g) charged domain walls by stacking them along the c-axis.

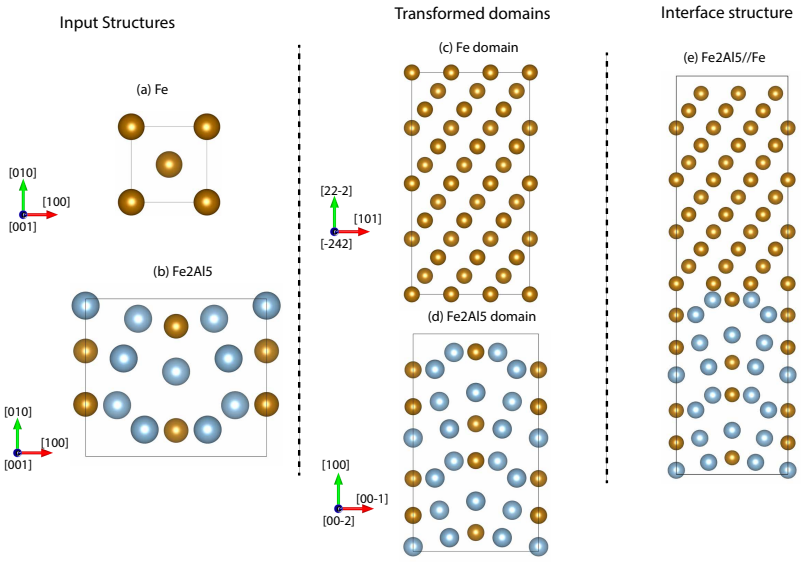

Figure 3: Illustration of the `hibuilder.py` script used to build the interface structures between (a) Fe and (b) Fe_2Al_5. The transformed bulk structures are shown in (c) and (d) respectively. The final interface structure is created by stacking the transformed bulk phases so that $Fe_{[22-2]}$ is parallel to $Fe_2Al_{5[100]}$. (e) The interface structure can be further optimized by defining the optimal distance between the two bulk phases.

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