Visualization of Barium Titanate Phase Transition using Quantization of Dipole Moment Vectors

Henry Lehmann   Patrick Heyne   Oliver Mothes   Heiko Müller   Tim Smyth   Erik Berger

Katja Fiedler   David Vogt   Bernhard Jung

TU Bergakademie Freiberg

{patrick.heyne,oliver.mothes,heiko.mueller,tim.smyth}@student.tu-freiberg.de
{henry.lehmann,erik.berger,katja.fiedler,david.vogt,jung}@informatik.tu-freiberg.de

ABSTRACT

In this paper we present our approach to visualizing a phase transition of barium titanate as contribution to the IEEE Visualization Contest 2012. The visualization is based on data sets from a molecular dynamics simulation of a barium titanate crystal comprising $625,000$ atoms. The scenario is a phase transition between paraelectric (cubic) and ferroelectric (tetragonal) phase. The goal of the visualization is to give insight into the evolution of polarization domains during 900 picoseconds of simulation time. The development of polarization domains is captured by vector quantization of dipole moments computed from the lattice cells. Due to strong thermal vibrations of the atoms, the domain evolution is quite noisy. This noise can be reduced through temporal smoothing and a clustering technique that allows for a small number of differently polarized cells within a domain. In this way, domains of reasonable size are identified and a global visualization of the phase transition is established.

1 INTRODUCTION

Simulation and visualization is an important methodology in prototyping and knowledge gain. As computational power becomes available physical phenomena in material science and biology can be studied in atomic scale for reasonable amount of elementary particles [7, 9] investigating molecular dynamics simulations [2]. However, due to the large amount of data, analysis and interpretation of the resulting movement of atoms is still a challenge and often requires individually designed software analysis tools [8, 5].

In the present case molecular dynamics simulation is applied to $BaTiO_3$ in the field of computational material science. Our approach to visualizing polarization domains in $BaTiO_3$ relies on temporal smoothing and quantization of dipole moment vectors of crystalline cells. Smoothing is incorporated to eliminate thermal vibrations from atoms movement and dipole moment vectors are used to define spatial regions of cells with similar polarization.

The remainder of this paper is structured as follows: In Section 2, we point out several aspects of the data set we encountered during first analyses. In Section 3, we explain the movement of the atoms and how the data is pre-processed for determining polarization domains. Section 4 explains our method for clustering of polarization domains. The results of our investigations are summarized in section 5.

2 FIRST IMPRESSIONS

The data consists of 500 time steps, which extend over a period of 900 picoseconds. Each time step contains position data for $625,000$ atoms, which makes a $BaTiO_3$ crystalline structure composed of $50 \times 50 \times 50$ crystal cells. Figure 4 *left* shows the whole structure, whereas figure 4 *top right* only shows one layer. Observing single atoms, their trajectories turn out to be very noisy. All atoms are subjected to heavy oscillations, coupled with an underlying movement towards the center of the crystal lattice. At first sight no special patterns can be recognized.

In material science literature, the relevant phase transition is described as relative displacement of atoms in a crystal cell. The paraelectric phase is given by a cubic cell structure, whereas the ferroelectric phase is given by a tetragonal structure [3, 4, 1]. The structures for para- and ferroelectric phase are shown in figure 5 *left* and *right* respectively.

The plots of figure 6 provide various evidence for the existence of a phase transition in the simulation data around time step 380. The atoms' velocities sharply increase and, similarly, the crystal volume (summed edge lengths of cells) starts to expand after contracting for most of the simulation. Similarly, the dipole moment of the crystal (summed magnitudes of cell dipole moments) decreases in the beginning of the simulation but increases again towards the end.

3 ATOM MOVEMENT

Atom displacement can be analyzed as superimposition of three movements: thermal vibration, lattice contraction, and cell deformation.

3.1 Thermal Vibration

The atoms' movement is heavily influenced by thermal vibrations. Figure 7 visualizes the vibrations of the atoms in a cell for a few consecutive time steps. In comparison to the displacement of the barium and titanium ions induced by the phase transition, thermal vibrations induce larger spatial fluctuations. During phase transition the cubic lattice is deformed along one axis by 1% [3]. In contrast thermal vibrations impose oscillations of about 5% of the cell's edge length.

To filter out thermal vibrations, temporal smoothing is applied. Smoothing is accomplished by applying B-spline regression to atoms positions. For each individual atom, positions are approximated by a least square B-spline [6] fit using equidistant knots and 50 control points. This gives a smooth curve, which follows the trend of atom's noisy movement as shown in figure 1. For a comparison of an original and a smoothed trajectory refer to figure 8.

3.2 Lattice Contraction and Expansion

Besides thermal vibration, atoms show movement towards the origin of the coordinate system. As can be seen in figure 6, lattice cells continuously contract until time step 410. In time steps 410 to 500 crystalline cells undergo a continuous expansion. In figure 9 this behavior is shown for titanium atoms in detail.

3.3 Cell Deformation and Dipole Formation

As noted above, the lattice cells change their shape during the considered phase transition. Due to the different cell shapes in the cubic and tetragonal phases, different cell polarizations arise.
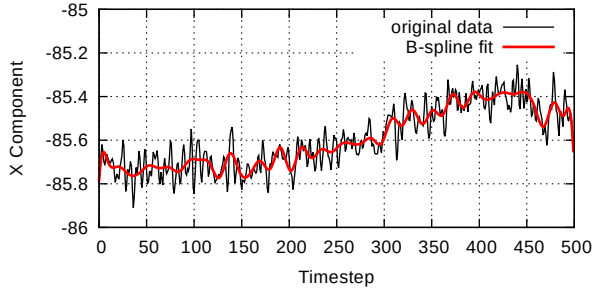
Figure 1: The plot shows the X component of position data of one single titanium atom for all 500 time steps. *Black:* original data. *Red:* smoothed data.

Polarization domains are determined by dipole moments of titanium centered crystalline cells. The dipole moment is given by the sum of the positions of Ba-, Ti- and O-atoms weighted by the atom's charge inside one cell. The resulting sum of the charge of one kind of atom additionally is weighted by the amount of cells, which share this atom. The dipole moment is calculated as follows

$$d = 4 \cdot p^{\text{Ti}} + \frac{1}{8} \cdot \sum_{i=1}^{8} 2 \cdot p_i^{\text{Ba}} + \frac{1}{6} \cdot \sum_{i=1}^{6} -6 \cdot p_i^{\text{O}} \qquad (1)$$

4 DOMAINS

To understand the evolution of polarization domains, we have to cluster neighboring cells with similar dipole moments. A difficulty results from the strong thermal vibrations of atoms, which also cause rapidly changing dipole directions of single cells (see figure 10). This noise can be reduced through temporal smoothing (cf. figure 1), dipole quantization, and a clustering technique that allows for a small number of differently polarized cells within a domain.
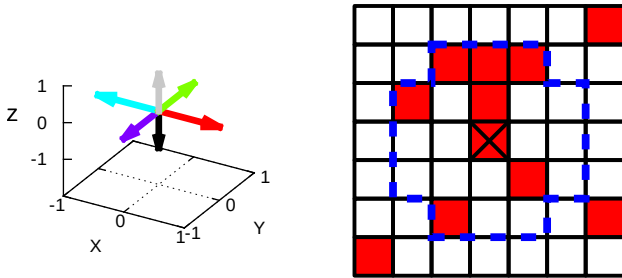

Figure 2: The six vectors (left) represent the quantized directions of the electric dipole moment. The grid (right) shows a cell in the center for which the neighborhood value is calculated within the blue line dotted region. In this case the neighborhood value equals 7.

Figure 2 (left) shows the six vectors used for quantization of dipole moments. Figure 11 shows slices through the crystal with cells colored according this quantization. Without further clustering, these patterns appear random and no domains can be detected by visual inspection.

Next, for each cell the number of neighboring cells with the same dipole quantization is counted. The neighborhood of a cell is defined as the set of lattice cells within a certain Euclidian distance to the considered cell. Figure 2 (right) illustrates the calculation of the neighborhood value.

Finally, cells are clustered into polarization domains. A cell is taken to be part of a domain, if its neighborhood value exceeds a threshold. Figure 12 shows the evolution of calculated domains with a parallel projection. Figure 13 gives an impression of domain evolution through a 3D view. Both visualizations indicate that domains are shrinking during the course of the simulation.

5 CONCLUSION

Due to the strong atom vibrations, the detection of domains based on atom positions only turned out to be quite challenging. In our approach, temporal smoothing with b-spline fitting and quantization of dipole moments are used to filter out these thermal vibrations. Using a clustering method based on counting similarly polarized cells in a cell's neighborhood, the evolution of polarization domains could be visualized.
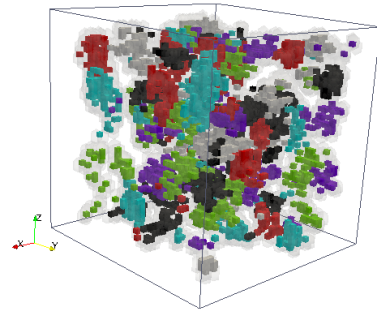

Figure 3: Visualization of quantized dipole domains.

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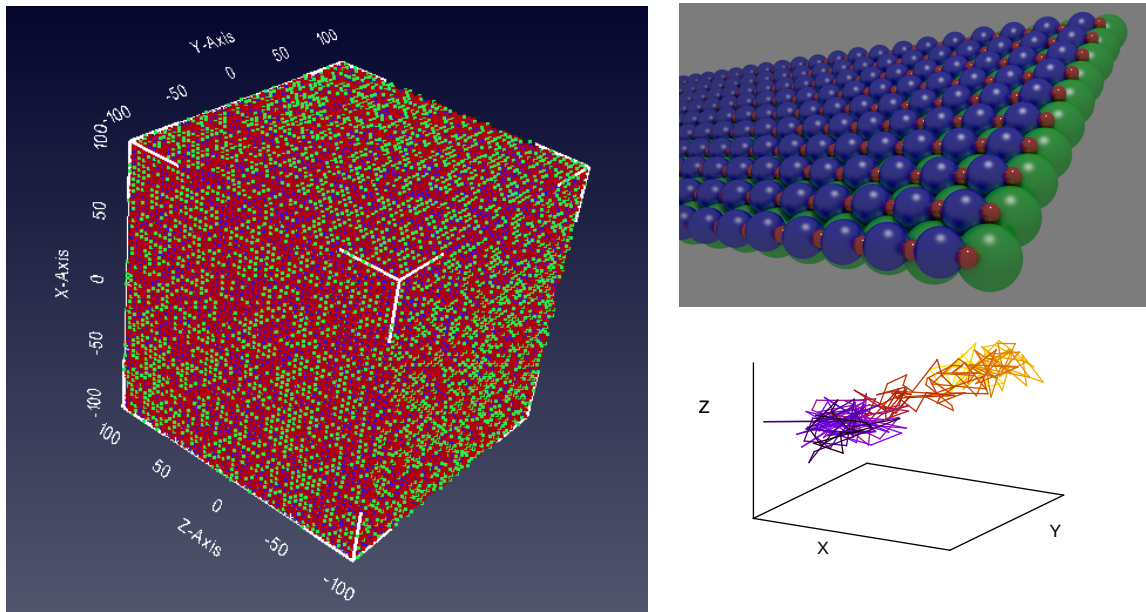
Figure 4: A first look at the simulation data. *Left:* the simulation grid with $50 \times 50 \times 50$ crystalline cells, with a total of 625,000 atoms. *Right top:* a single layer. *Right bottom:* trajectory of a single atom over 500 time steps.
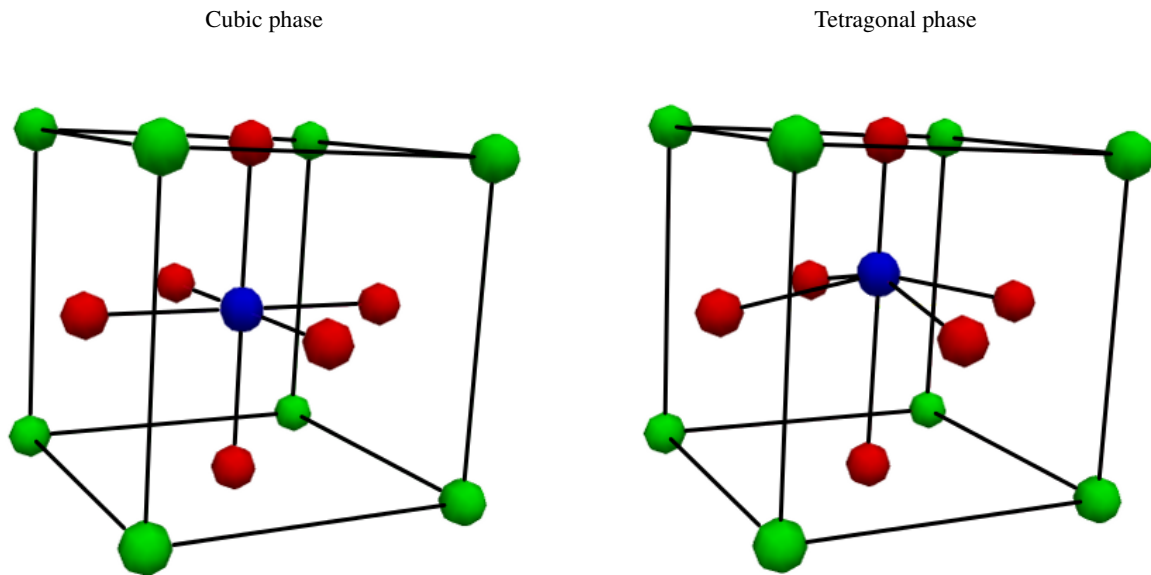
Cubic phase   Tetragonal phase

Figure 5: Idealized illustration of cubic and tetragonal $BaTiO_3$ phases (Ba *green*, Ti *blue* and O *red*). *Left:* cubic phase of a titanium centered crystal cell. *Right:* tetragonal phase. Ti-atom is displaced w.r.t. the O atoms. As the Ti atom is charged positively and O-atoms negatively, a dipole moment is created along the up-direction.
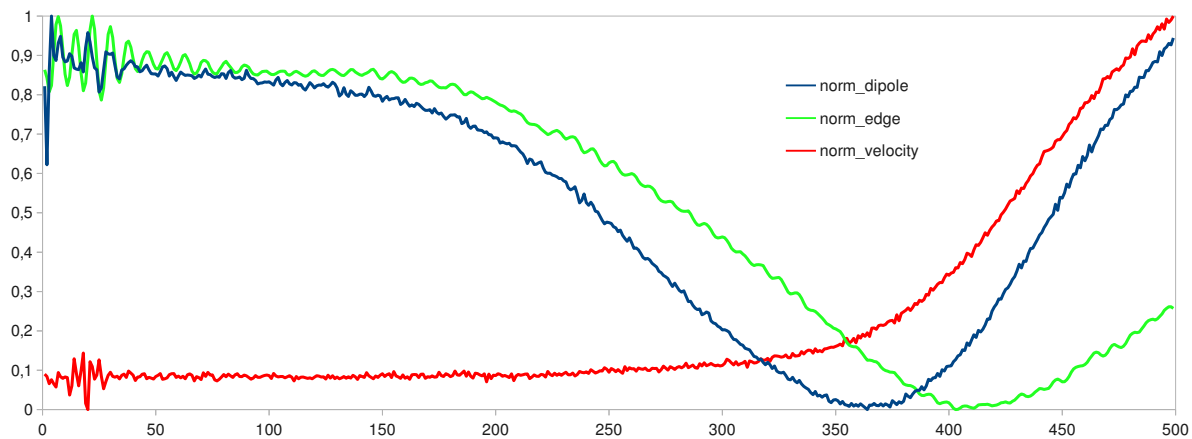
Figure 6: Global view of the dataset: This plot shows the magnitude of the dipole moment, edge length of crystal cells and magnitude of velocity vector for each time step averaged over the whole data set.
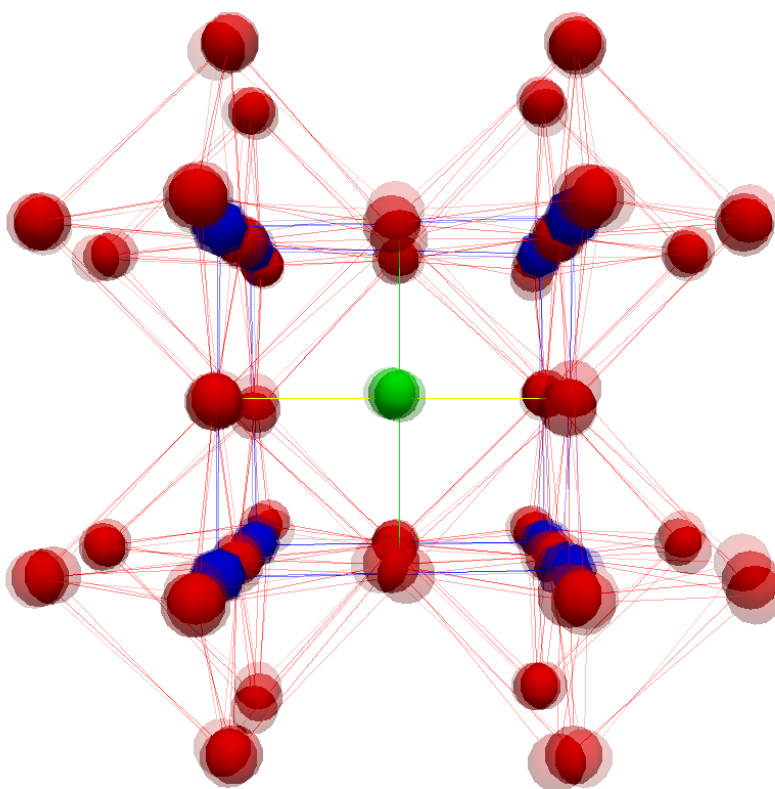

Figure 7: Thermal vibrations inside barium centered crystal cell. Fluctuations of atoms' positions are shown by transparent crystal cells.
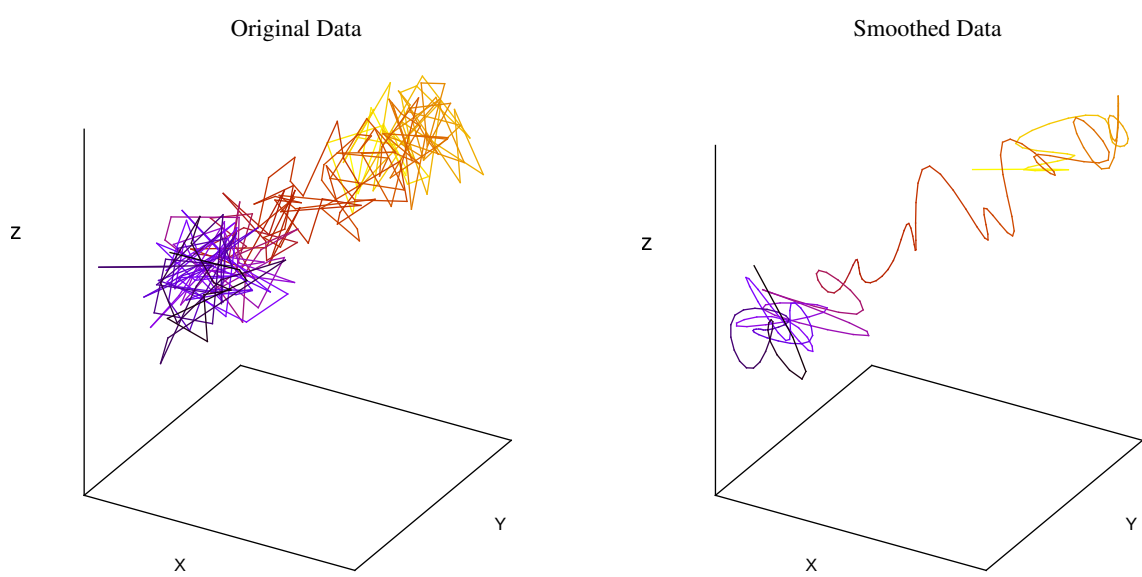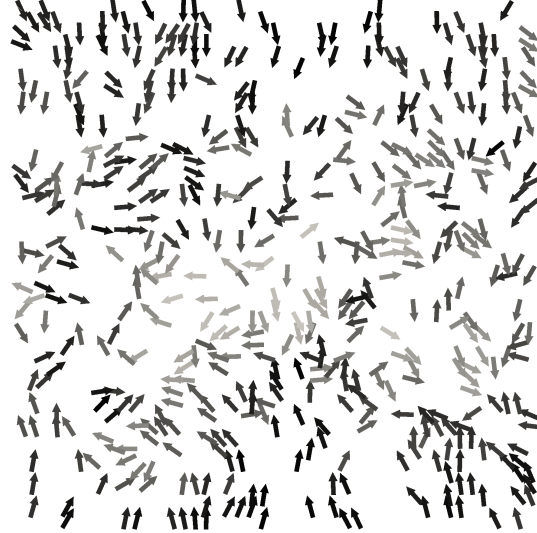
Figure 8: Impact of smoothing atoms' trajectories: *Left:* original data. *Right:* Resulting trajectory after applying B-spline regression.

Time step 245 to 295

Time step 295 to 345

Time step 370 to 420

Time step 445 to 495

Figure 9: Lattice contraction and expansion: During the simulation, contraction and subsequent expansion is observed. Until time step 400, atoms mainly move to the center of the coordinate system which downsizes crystal cells. In time step 400 to 500, atoms tend to move away from the center of the coordinate system which enlarges crystal cells.

Time step 75

Time step 215

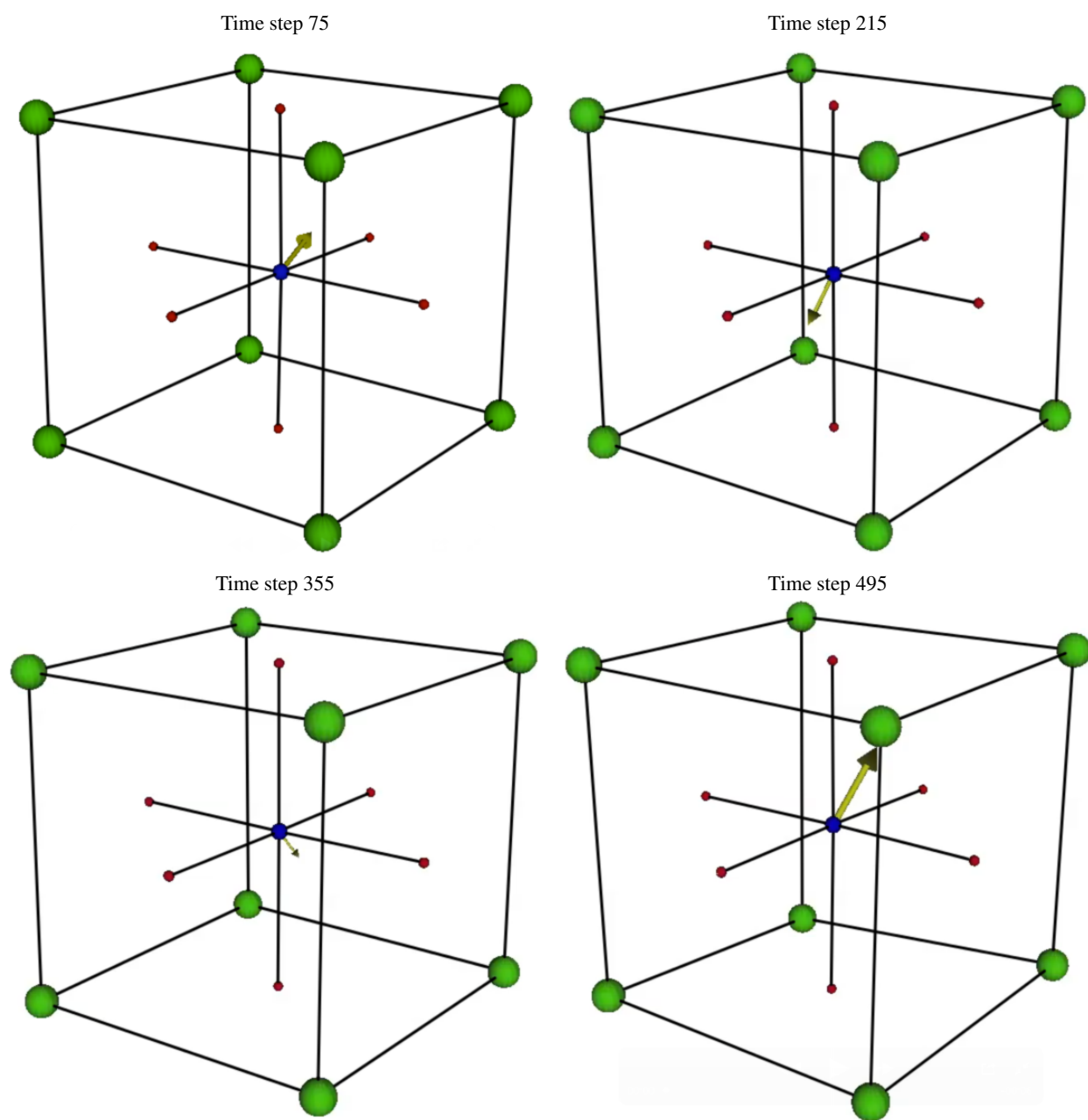Time step 355

Time step 495

Figure 10: Dipole moment of a titanium centered crystal cell shown at time steps 75, 215, 355 and 495.
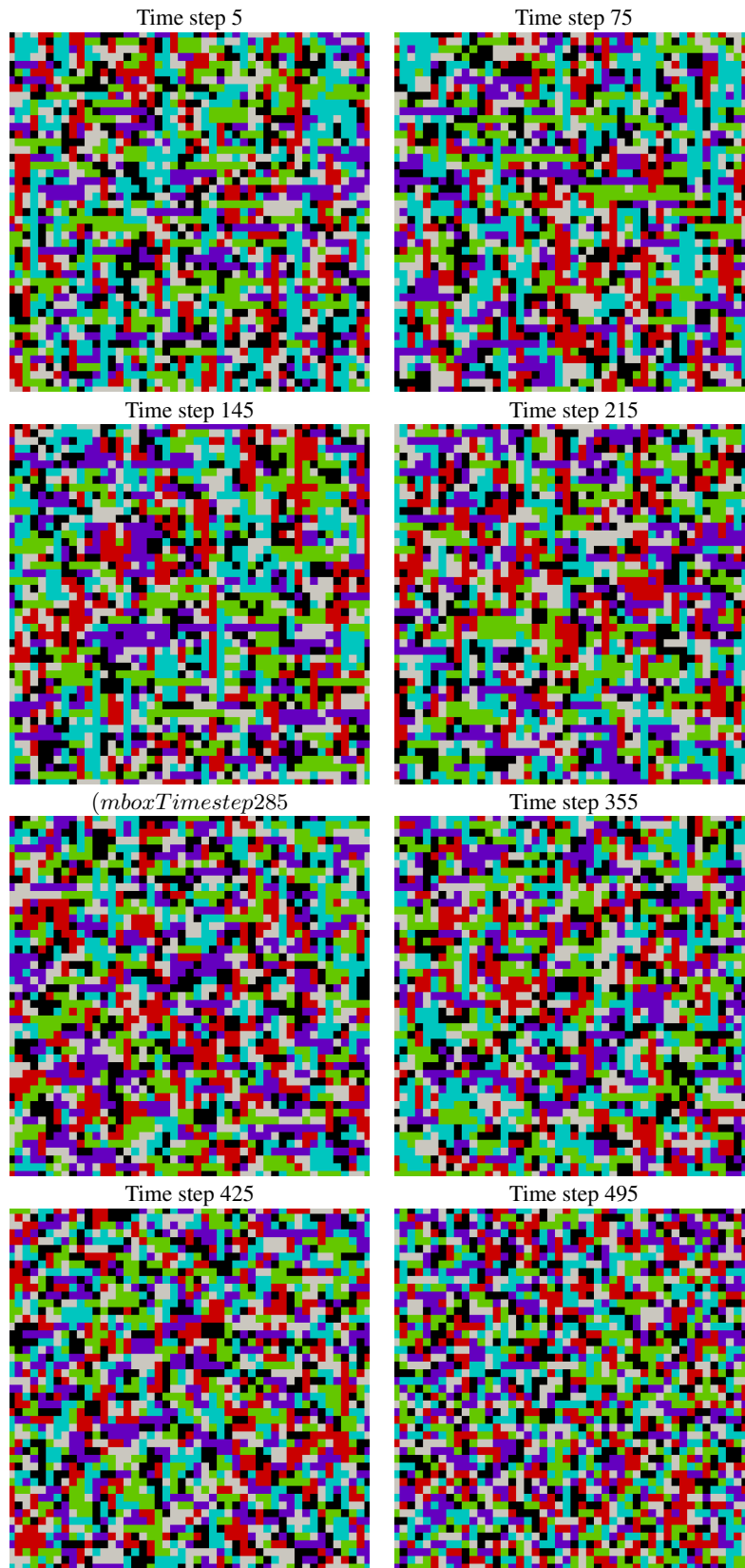
Figure 11: One slice of quantized dipole moment vectors of titanium centered crystal cells shwon for time steps 5, 75, 145, 215, 285, 355, 425 and 495. Dipole moments are mapped to six directions, which is illustrated by different colors.
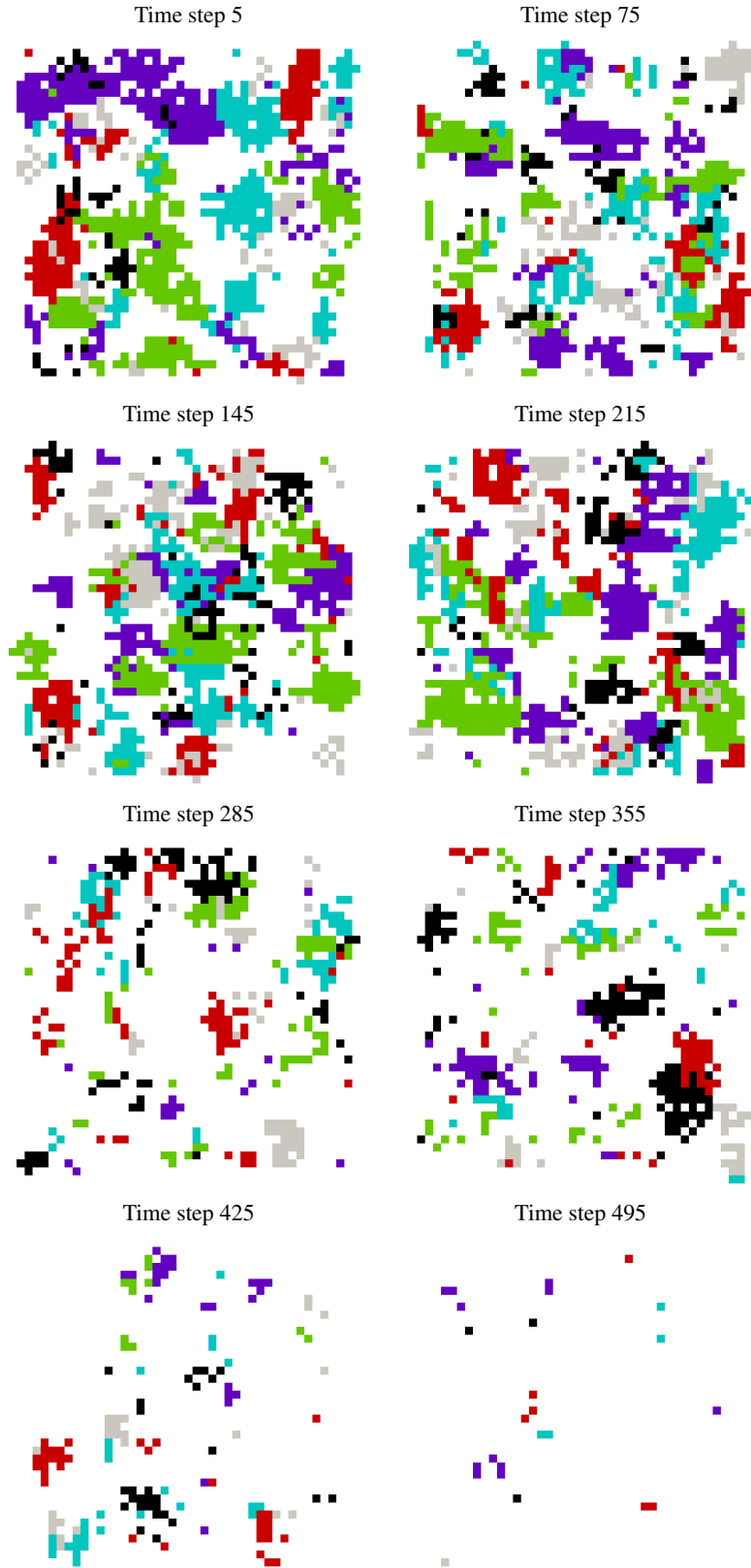
Figure 12: Neighborhood value calculated from quantized dipole moments for time steps 5, 75, 145, 215, 285, 355, 425 and 495. The color corresponds to quantization direction. Neighborhood value is calculated using a distance of $d = 4.5$. Only cells which have a neighborhood value greater or equal to 90 are shown to determine polarization domains. The plots are shown in parallel projection along the z-axis.

Time step 5

Time step 75

Time step 145

Time step 215

Time step 285

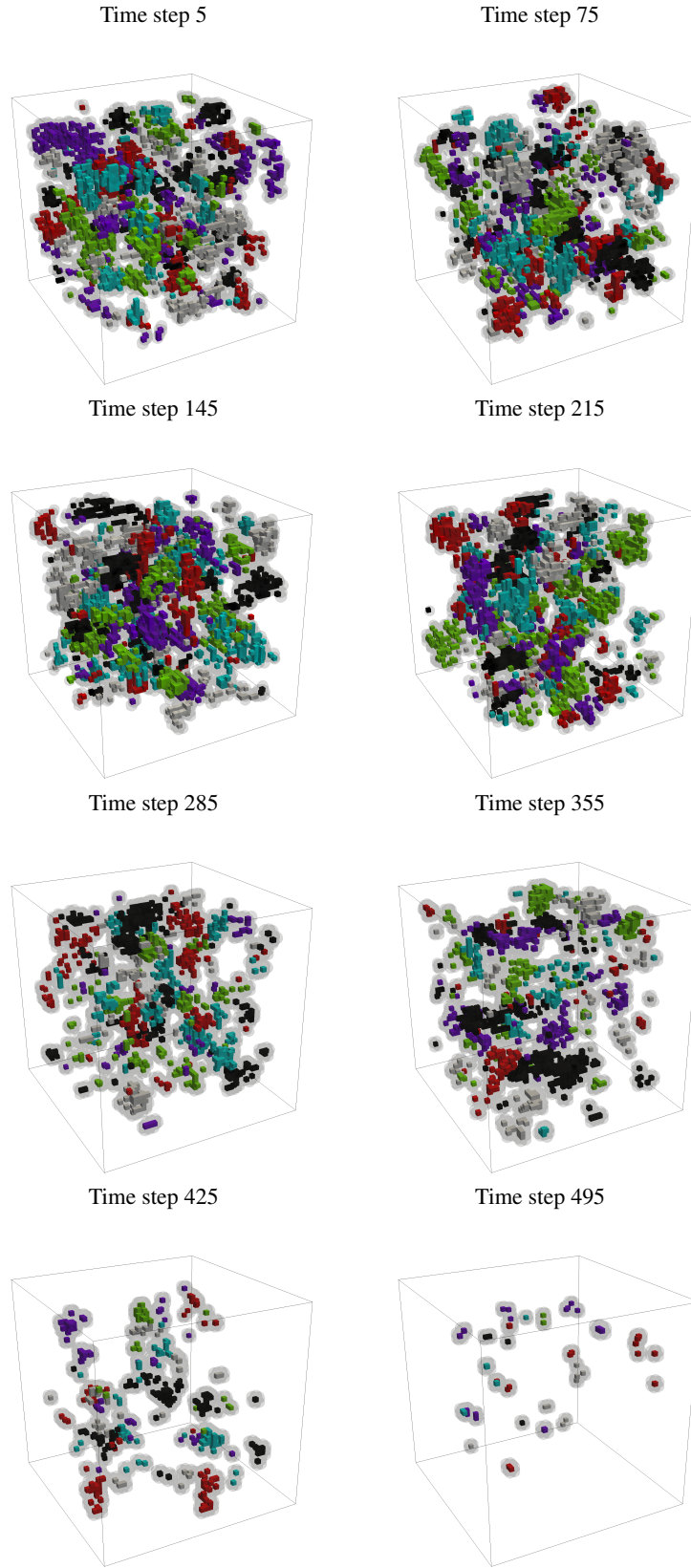Time step 355

Time step 425

Time step 495

Figure 13: Neighborhood value calculated from quantized dipole moments for time steps 5, 75, 145, 215, 285, 355, 425 and 495. The color corresponds to quantization direction. Neighborhood value is calculated using a distance of $d = 4.5$. Only cells which have a neighborhood value greater or equal to 90 are shown to determine polarization domains.