Three-Dimensional Visualization of Atomic Collision Cascades

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Abstract. The paper describes a new approach to the visualization of atomic collision cascades and using the interaction with visualized data. The collision cascade is a physical phenomenon initiated by bombarding the surface of a solid with accelerated atomic particles. The process evolves in time and therefore it is necessary to develop some tools that would allow to investigate and visualize the dynamics of the process. Such tools are classifiers (filters) that enable to select and visualize objects with specific dynamic properties. As the visualization has been done in a 3D environment a question arises how to specify effectively and user friendly both the properties and the objects in the 3D space. Several techniques are available that allow interaction in the 3D space. It has been necessary to test some of these techniques and to determine which one is the most suitable for the given application class.

1 Introduction

A simulation of real physical systems is usually a time consuming problem connected with a tedious visualization task. Many such physical systems are described by a set of time dependent differential equations. Using computers we are able to solve these equation sets and afterwards we may visualize the results so that scientists can get a better insight into the studied physical processes. The problem we have been solving is a non-linear molecular-dynamics system with a large number of first-order differential equations. Dynamic systems are in general described by $\frac{d\boldsymbol{X}}{dt} = \boldsymbol{F}(\boldsymbol{X}, \boldsymbol{\alpha}, t)$ equations where $\boldsymbol{X} \in \mathbb{R}^n$ of the n-dimensional phase space, $\boldsymbol{\alpha}$ are system constant parameters and t is the time. By solving these equations we obtain $\boldsymbol{X}(t)$. The equations can be only solved by means of numerical methods. The dimension n of the phase space as of $\boldsymbol{X}(t)$ is usually very high and a projection into a less-dimensional space is inevitable, e.g. visualization of molecular-dynamics would be a projection into a 4D space (3D Euler's space and time parameter). In Sect. 2 we discuss the molecular-dynamics and its computer simulation in more detail. Section 3 describes our approach of molecular-dynamics visualization with two-level classifiers that help to reduce the number of visualized data. Special attention has been paid to the handling of dynamic attributes of the visualized objects. Section 4 describes our experiment that enables to compare the effectiveness of the interaction in different display modes. In the implementation we have restricted ourselves to common

visualization devices; anaglyph glasses, shutter stereo glasses as view devices and a common mouse device as an 2D input device. We did not work with more advanced and more expensive VR tools.

2 Physical Background of the Problem

The physical phenomenon in our case could be shortly described as follows. The surface of a solid e.g. aluminum is bombarded with accelerated ions or neutrals. During the collision the accelerated particle interacts with atoms of the solid and knocks some of them out of the surface. This dynamic process is called the *collision cascade*. The scientists are especially interested in the way how the surface atoms are knocked out (the process is called the atomic *sputtering*), in which direction they are emitted and what kinetic energy they have. The information on sputtered particles is of a significant importance in several surface analytical techniques, in techniques used for cleaning of solid surfaces and in modern technologies based on ion induced chemical processes (e.g. mechanical hardening of polymer surfaces). Also of the interest is the average distance which the bombarded particles travel in the solids. The knowledge of this range is of great practical interest in the technological process called implantation in which impurity atoms are implanted in semiconductors to change their resistivity in a controlled way or into metals to change their mechanical properties.

Dynamic properties of particles are in general described by a second-order differential equation of the following form

$$\boldsymbol{F} = m\frac{d^2\boldsymbol{r}}{dt^2} = -\mathrm{grad}\,\varphi\,, \tag{1}$$

where $\boldsymbol{F}$ is the force acting on the particle, m is the particle mass, $\boldsymbol{r}$ is the position vector and φ is the potential at the point $\boldsymbol{r}$. The potential φ describes how the particles interact with each other. The precision of the simulation depends critically upon a proper choice of this potential. The simplest is the *binary potential* which depends only upon the particles between which it is calculated and on the distance between them. It is independent of positions of the other particles. The potential function is usually a composition of more than one function joined together, each of which is valid only within a specific distance interval. The value of the binary potential is significant only within the certain radius and outside this radius it is assumed to be zero (a finite cut-off radius). Some examples of binary potential could be find in [1] and [2]. The (1) describes the dynamic properties of one particle and could be split into 6 simple first-order equations of the type $\frac{d\boldsymbol{v}_i}{dt} = -\frac{1}{m_i}\frac{d\varphi_i}{d\boldsymbol{r}}$ and $\frac{d\boldsymbol{r}_i}{dt} = \boldsymbol{v}_i$, where $\boldsymbol{v}_i$ is the velocity and $\boldsymbol{r}_i$ is the position vector of the i-th particle. In our case we investigate the collision cascades produced by relatively low energy primary particles (< 1 keV). It turns out that for such low impact energies the collision cascades occupy a small volume and thus clusters typically 10x10x10 atoms are sufficient. The number of equations to be solved is then around 6000. The dynamic process is over in about 200 fs after the impact of the primary particles. For the purpose

of the simulation we have implemented a one-step numerical method for solving first-order equations called *Runge-Kutta* with Gill's modifications [5] [6] (we call the program **SPUTT**).

2.1 Statistics

In actual experiments, when the surface of solids is bombarded with accelerated particles, the surface is not hit exactly at the same place several times. Instead, we have a stream of accelerated particles, which collide with a large area of the surface. On the other hand in the software simulation of collisions (in the **SPUTT** program) the particle hits the surface precisely at the point given by the user. For a single crystal with a perfect surface at temperature zero, the surface crystallographic structure defines an *irreducible surface element*. Using the symmetry and translation invariance of the surface, the ion bombardment into this irreducible surface element is representative of the ion bombardment of the entire surface. So we solve the collision cascades for different impacts on a regular grid in the irreducible surface element. We have denoted the obtained collision cascades as a *collision cascade set* (**CCS**).

2.2 Simulation Time Requirements

To give an example of the computing time of common problems the simulation of a 10x10x8 Al cluster bombarded with 560 eV Ar ion at 1000 different impact points took 48 hours on IBM RS6000 workstation. There are several techniques how to reduce the computation time of the simulation. Firstly, the number of atoms with which any particle interacts is finite due to the fact that we have a finite cut-off radius of the potential. Since the identity of the interaction partners changes with time as a consequence of particle motion, neighbor lists are used. The best list nowadays in use is the Verlet-linked-cells algorithm [7]. Secondly, it is preferred to encode potentials as look-up tables rather than as analytical expressions to be evaluated. Thirdly, the numerical method for solving differential equations can take advantage of determining a local error in each time step and appropriately increasing or decreasing the time step. Implementing all three techniques we may reduce the computation time by a factor of 10.

3 Visualization of Molecular-Dynamics

Visualization is an essential part of many dynamic system simulations. The molecular-dynamics simulation of sputtering as it was described above is not an exception. Information about the sputtered yield are of a great importance and most of the scientific monographs concerning the molecular-dynamics provide a statistical analysis of simulated data and then compare obtained results with laboratory experiments. Some of the common analyses are: the distributions of the sputtered yield within the irreducible surface element (see Sect. 2.1) [3], the energy and polar-angular distributions of sputtered particles [1], etc. Direct

visualization of the bombardment is often presented in these monographs in the form of static images of collision cascades before and/or after the bombardment, see [3] and [4].

We have aimed our research at a direct dynamic visualization of collision cascades *CASVIS* (*CAS*cade *VIS*ualization), i.e. we track and display individual particles in time during collisions. Dynamic visualization of CCS as a whole would inevitably involve special statistical approaches that would project collision cascades in CCS into some more comprehensive data. One of the approaches could be to display "temperature" distribution in CCS as a function of time and thus be able to track the "*hot spots*" (areas of high activity). Here the "temperature" $\mathcal{T}(\boldsymbol{r}, t)$ at a certain point $\boldsymbol{r}$ and time t could be defined as a mean value of energies of particles averaged over all collision cascades in CCS located at time t in an area around point $\boldsymbol{r}$. This approach is in a stage of development and we want to cover it in our future work. Iconic techniques [10] that display particular parameters at given points of a more complex visualization procedure may be of a great benefit here, e.g. by displaying sputter yields at specified points.

Up to now, we visualize collision cascades in CCS separately and we have not implemented any statistical procedures. Unfortunately this technique may obscure some features otherwise observable in statistical approaches, but on the other hand it gives a precise insight into dynamic properties of individual collision cascades. We know that some impacts trigger dramatic sputter activities and such processes are only observable by visualizing suspected collision cascades. Knowledge of atomic-dynamics during coincident collision cascades, when sputter and scatter phenomena occur simultaneously, is of a great importance for scientists. Such cascades are selected from CCS and properly visualized only by means of classifiers.

3.1 Classifiers

As we have seen in Sect. 2.2 one CCS consists of 1000 collision cascades each for one cluster of around 1000 particles. We face a common problem in the scientific visualization of physical processes, i.e. we are overwhelmed by a vast number of data. Use of adjustable software classifiers that assort collision cascades in CCS is thus convenient. Two level classification is proposed in this paper. Classifiers of the first level, i.e. the *cascade classifiers*, are designed to extract collision cascades from CCS that match some given specification. Classifiers of the second level, i.e. the *particle classifiers*, are intended to select (emphasize) "interesting" particles in the visualized collision cascade. By the word "interesting" we mean particles that match certain conditions.

Applying cascade classifiers on CCS produces a *collision cascade subset*. An example of two cascade classifiers follows:

- **Select collision cascades with a certain sputter yield.**
  We can, for example, select cascades with a high or a low sputter activity, or select cascades in which only certain particles of the cluster are sputtered.

– **Select collision cascades in which impact particles penetrate to a certain depth of the cluster.**
  We can, for example, determine cascades in which an accelerated impact particle bounces off the cluster surface, i.e. the impact particle is *scattered* by the cluster.

An efficiency of the cluster classifier can be designed as $1-(N_{sel}/N_{all})$, where N_{all} is the number of all collision cascades in CCS, and N_{sel} is the number of cascades in CCS selected by the classifier. The efficiency depends completely on the type of the cluster classifier and on the type of CCS. Currently we have implemented one cluster classifier that selects clusters in which an impact particle bounces off the surface. Applying this classifier on CCS containing 450 collision of a 945 eV Li ion with an Al cluster has led to 255 matches.

The particle classifiers are included in the user-interface of our visualization system CASVIS. So far we have implemented two particle classifiers in the following way:

– **Select particles with energies above a certain threshold**
  This way we select particles which will move faster than the specified threshold of the kinetic energy. CASVIS features an easy setting of the threshold with a scrollbar widget. In Fig. 2 we see the result of this classifier. Particles that match the classification are drawn as spheres and the rest as dots.
– **Select particles that will pass through a certain plane**
  If we set the plane above and parallel to the cluster surface we select particles that will be sputtered through that plane. CASVIS enables easy manipulation of the plane by moving and rotating the qplane object. In Fig. 3 we see the selected particles drawn as spheres and the plane object.

In CASVIS users can interactively set parameters of the classifiers and thus dynamically modify the visualization output according to the users' needs, i.e. the given approach allows us to describe interactively some dynamic properties of the visualized objects. These properties form a special class of classifiers (filters) that help to visualize the dynamics of the process in certain context and thus lead to better understanding of the visualized physical phenomenon. It is obvious that the setting of classifier parameters requires an intensive interaction in 3D space due to the 3D nature of classifier characteristics.

3.2 Features of CASVIS

In our case of the many-particle problem we do not have to solve issues connected with visualization of vector or scalar fields, although the potential field created by particles is of a scientific interest and in our future work we want to implement it. We perceive individual particles as points in space that behave according to well defined rules, see Sect. 2 and therefore we have decided to represent them simply as spheres. CASVIS implements three different 3D display modes: *perspective viewing*, *anaglyph stereo* and *shutter glass stereo*, as follows:

- **perspective viewing**
  A perspective projection transformation is applied to the image data (a position of particles). Particles are projected onto a 2D plane in color. No additional hardware is required.
- **anaglyph stereo**
  Two perspective views of clusters are generated; for right and left eye with complementary colors (red/blue or red/green). 3D perception is achieved through anaglyph glasses with filters in complementary colors. The serious disadvantage of this method is the lack of color information. This information is only partially present in shades of grey.
- **shutter glass stereo**
  Two perspective views of clusters are generated using the same color scale as in the perspective viewing. The right and left eye views are presented alternatively on the screen.

CASVIS behaves identically under all three display modes. We restricted ourselves to 2D input device mouse and use a so called *laser beam* [11] to assist interaction in the 3D scene. The beam is a ray, cast from the user's pointer in a straight line perpendicular to the screen plane. The first object to be intersected by the ray is selected for manipulation. This way users can drag and rotate the particle cluster in space and select particles. In this manner selected particles display their current position and energy. Due to a large number of displayed particles, we have decided to plot selected particles as spheres and remaining ones as dots. This technique dramatically improves the perception because significant areas are emphasized. To improve and speed up the selection a selecting technique of *particle classifiers* introduced in Sect. 3.1 was implemented, e.g. pick up particles with energies above a specified threshold (Fig. 2) or pick up particles that were sputtered (Fig. 3). Colors are used to distinguish between different kinetic energy levels of particles. Kinetic energies are mapped into a color spectrum and the mapping can be adjusted arbitrarily. Finally trajectories of selected particles can be also included in the image. Users can track the cascade development by changing the time manually or by turning on an animation sequence. In Fig. 4 we have shown the collision cascade 140 fs after the impact.

4 Psychological Test of the Interaction Effectiveness in Different Display Modes

Up to now we were mainly concerned with the question how to map simulated data to meaningful images that would help to understand collision cascades. One of the interesting issues connected with it is the effectiveness of a particular interaction technique in a specific display mode. This issue is in general very broad and complex. Many experiments were proposed in the past and carried out in different environments and with emphasizes on different tasks.

Unfortunately, up to now, only a static perception of visualized 3D objects was performed. In [8] images of chemical molecules were used and volunteers

(subjects) were asked to perform three different tasks (identifying, comparison, movement) under three different display modes (perspective, anaglyph stereo, shutter glass stereo). Two interesting conclusions were reached. Firstly, if the third dimension doesn't provide any necessary information the interpretation of the visualization is more difficult. Secondly, the viewing in the anaglyph mode is as good as in the shutter mode. Presented with a pair of object images, the subject's task in [9] was to determine whether the two images represented the same or different objects. One of the interesting results was that the accuracy of the subject's task was significantly improved when the object motion was controlled. However the response time of the subject's task was longer.

4.1 Experiment

The above described experiments were of passive nature. In our study subjects, besides the image interpretation, performed also the *interaction* in 3D. The purpose was to evaluate the effectiveness of three display modes for different interaction tasks. These interaction tasks were selected as typical for the given application. CASVIS system discussed in Sect. 3 served only as an experimental environment. The scientific interpretation of images was not considered in our experiment. The experiment involved 20 subjects who were students of Computer Science and had more or less the same experience with the 3D representation. The tasks were performed interactively on each of the 3D display modes (perspective, anaglyph stereo, shutter glass stereo). Presented with a cluster of particles (spheres) positioned in 10x10x8 cube, the subject's tasks were the following:

1. set the "plane" object parallel to the larger cube sides,
2. selecting individual particles define 2x2x2 cube in one corner of the 10x10x8 cube,
3. count selected particles (spheres) in the cube.

As an interaction tool, the mouse with a *laser beam* selection technique was used, see Sect. 3.2 for a detail description. Tasks were designed to take the advantage of the classifiers and to emphasize different domains; task 1 should emphasize the object manipulation in space, task 2 the object selection in space and task 3 the identification of objects. In all the cases the subjects were allowed to rotate the cluster in order to improve the accuracy [9]. We were aware of the fact that the subjects could improve their performance during testing because they can find (learn) more efficient procedures how to reach the desired output of the tests. To reduce the influence of this learning parameter we allowed the subjects to perform the tasks more than once before measuring their response time. The accuracy of a subject's response was measured for task 1 and 3 only.

4.2 Results and Discussion

The results of the experiment should show in which display modes the 3D interaction is the most suitable to solve the particular task. Table 1 summarizes

Table 1. Mean response time $\bar{t}$ and mean response error $\bar{e}$ of 20 subjects for three different tasks and three display modes. F and p-value were computed by a one-way Analysis of Variance (ANOVA) and are defined in [12]

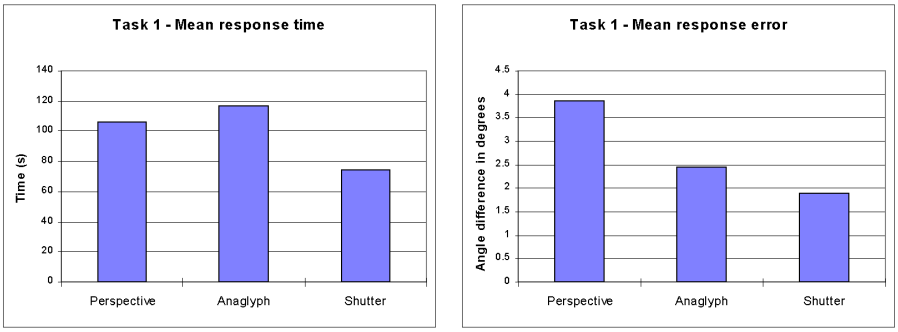
	mean response	Persp.	Anaglyph	Shutter	$F(2,57)$	p-value
Task 1	$\bar{t}(s)$	105.87	116.87	74.25	4.36831	0.01636
	$\bar{e}(degrees)$	3.84	2.45	1.88	2.72328	0.07272
Task 2	$\bar{t}(s)$	27.37	40.12	26.75	2.09214	0.13118
Task 3	$\bar{t}(s/sphere)$	1.16	1.17	0.94	1.00434	0.37158
	$\bar{e}$(mismatched counts)	0.5	0.37	1.75	5.28571	0.00867

the main effects of display modes obtained from our psychological test. Mean response times and mean response errors are plotted in Fig. 1 for individual tasks. F and p-value were computed by a one-way Analysis of Variance (ANOVA) for $\alpha = 0.05$. A detailed discussion of the statistical quantities can be found in [12] and will not be covered in our paper.

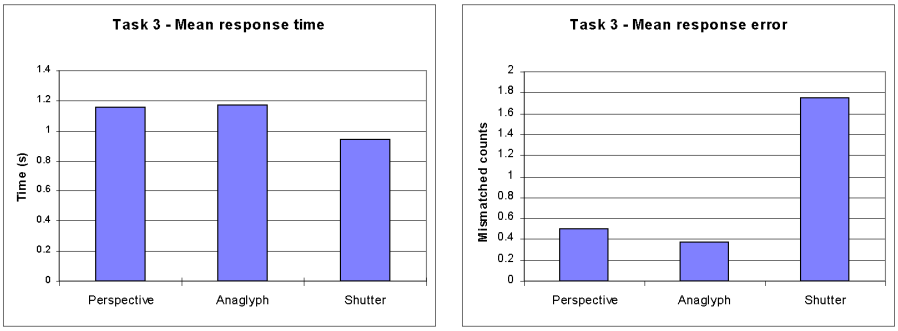
In task 1 the display mode has a significant influence on mean response times and mean response errors; p-value < 0.1 was found in both cases. The object manipulation in the shutter mode was performed more accurate and faster than in the perspective and the anaglyph modes, see Figs. 1(a), 1(b)). According to a Scheffé test [13] only the mean response time in the shutter mode was significantly better than in the anaglyph mode. This was an expected result.

Mean response times of task 2 and task 3 are not significantly influenced by the display mode (p-value > 0.1). So the observation (see Table 1 and Fig. 1(c)) that the shutter and the perspective modes are faster than the anaglyph mode for object selection and identifying is only a trend and not a significant result. On contrary counting of spheres in task 3 was significantly more accurate in the anaglyph and the perspective modes than in the shutter mode as the Scheffé test [13] indicated (see Fig. 1(d)). Results obtained from task 3 correlate with the results in [8], where the authors conclude that display modes have no significant influence on mean response times for counting rings in simple molecules. In our task 3 images consist of around 35 spheres and that was probably of similar complexity as images of simple molecules in [8]. Moreover, from task 2 we deduce that the same conclusion holds also for the object selection.

It is obvious, from the obtained results, that the 3D interaction is the most effective in the shutter display mode, but the 3D perception could be blurred in this mode. Furthermore the 3D interactive control of scientific visualization environment improves both understanding and manipulation with visualized objects. Therefore the investigation of new 3D interactive controls in scientific visualization may introduce desired positive effects. We believe that the particle classifiers introduced in Sect. 3.1 are the good example of such interactive controls.



(a) (b)



(c) (d)

Fig. 1. Mean response times (in seconds) for task 1 - 1(a) , mean response errors (deviation of plane normal from correct orientation in degrees) for task 1 - 1(b); mean response times (in seconds/one sphere) for task 3 - 1(c), mean response errors (number of mismatched counts) for task 3 - 1(d)

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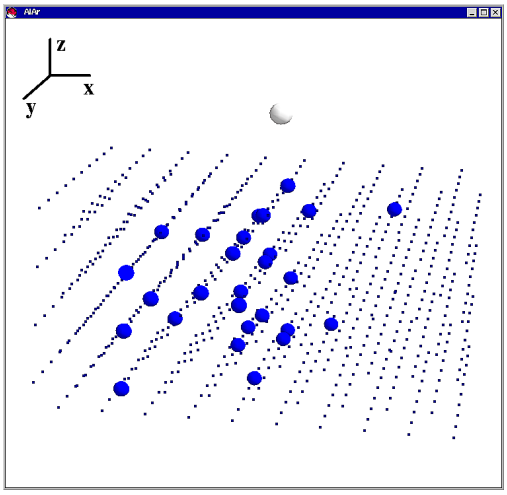

Fig. 2. The Al cluster before the impact of the 555 eV Ar ion (the lighter sphere in the upper part of the image). The ion is moving along the z axis. The Al atoms of the cluster are shown as black dots. Those Al atoms which will move later during the collision with kinetic energies larger than 10 eV are shown as dark spheres and are selected by the *energy particle classifier*. The image was produced by CASVIS in the perspective display mode.

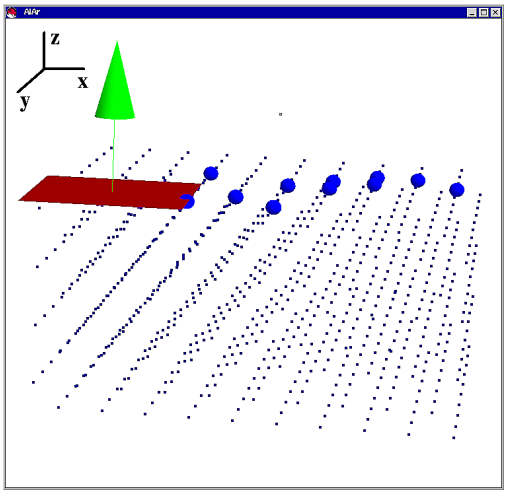

Fig. 3. The Al cluster before the impact of the Ar ion (555 eV) as in Fig. 2. Particles, displayed as spheres, will sputter later in the collision cascade and are selected by the *plane particle classifier*. The plane object is the rectangle with the normal vector. The image was produced by CASVIS in the perspective display mode.

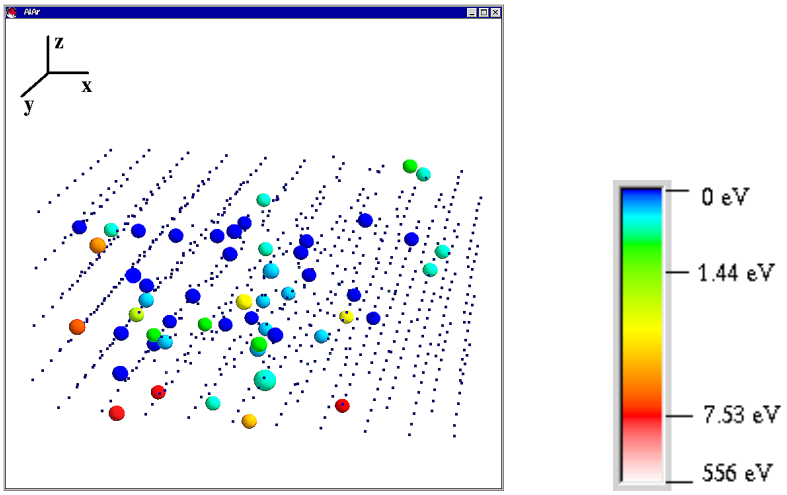

Fig. 4. The Al cluster 140 fs after the impact of the Ar ion (555 eV). The image was produced by CASVIS in the perspective display mode. The *energy particle classifier* is set to 5 eV. Color mapping of kinetic energies is according to the color bar on the right.