



HAL
open science

Molecular dynamics study of roughness and stress evolution using a Lennard–Jones potential

Tomasz Adam Zientarski, Dariusz Chocyk

► **To cite this version:**

Tomasz Adam Zientarski, Dariusz Chocyk. Molecular dynamics study of roughness and stress evolution using a Lennard–Jones potential. *Molecular Physics*, 2007, 105 (23-24), pp.3099-3107. 10.1080/00268970701762578 . hal-00513160

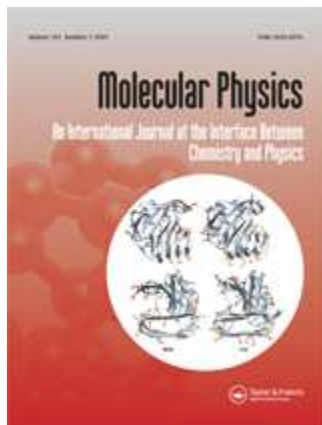
HAL Id: hal-00513160

<https://hal.science/hal-00513160>

Submitted on 1 Sep 2010

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Molecular dynamics study of roughness and stress evolution using a Lennard--Jones potential

Journal:	<i>Molecular Physics</i>
Manuscript ID:	TMPH-2007-0235.R1
Manuscript Type:	Full Paper
Date Submitted by the Author:	17-Oct-2007
Complete List of Authors:	Zientarski, Tomasz; Maria Curie-Skłodowska University, Department for the Modelling of Physico-Chemical Processes Chocyk, Dariusz; Lublin University of Technology, Advanced Materials Engineering Research Group
Keywords:	film growth, stress, roughness, molecular dynamics simulation
<p>Note: The following files were submitted by the author for peer review, but cannot be converted to PDF. You must view these files (e.g. movies) online.</p> <p>ZientarskiPaperMolPhys.tex</p>	



1 *Molecular Physics*, Vol. 00, No. 00, DD Month 200x, 1–16
2
3
4
5
6
7
8

9
10 **Molecular dynamics study of roughness and stress evolution using**
11 **a Lennard–Jones potential**
12
13

14
15
16 T. Zientarski*† and D. Chocyk‡
17

18 †Department for the Modelling of Physico-Chemical Processes, Maria Curie-Skłodowska
19 University, ul. Gliniana 33, 20-614 Lublin, Poland
20
21

22 ‡ Advanced Materials Engineering Research Group (AMERG), Lublin University of
23 Technology, ul. Nadbystrzycka 38, 20-618 Lublin, Poland
24
25

26
27
28 *(Revised reprint submitted to *Molecular Physics* October 17, 2007)*
29

30
31 A three-dimensional molecular dynamics simulation (MD) is proposed to study the film
32 growth, roughness and stress evolution during atoms deposition on the (100) plane of a fcc
33 regular crystal. We use cubic system with x-y periodic boundary condition. At the bottom
34 we have an atomic surface and at the top a reflecting wall. The model uses the Lennard-
35 Jones potential to describe the interatomic forces. The simulation results show that the film
36 grows with the Volmer-Weber mode and exhibits specific curve shape of the stress evolution.
37
38 The mean biaxial stress obtained during the simulation attains a local tension maximum
39 at a coverage of two monolayers. The stress in normal direction is smaller than the biaxial
40 stress. The main contribution to the stress in the film arises from the first monolayer. The
41 curves describing roughness possess maximum values at the same substrate coverage. The
42 dependence of the roughness on the temperature is examined.
43
44
45
46
47

48 *Keywords:* film growth; stress; roughness; molecular dynamics simulation
49
50
51
52
53
54
55
56

57
58

*Corresponding author. Email: martom@dyzio.umcs.lublin.pl
59
60

1 Introduction

Stresses are usually generated during the process of thin films deposition independently of the deposition technique applied and one can influence the reliability of evaluation of the deposited system properties by applying appropriate techniques. In some case, system properties of strained films can be improved. In other, stresses can lead to defective functioning, or even to breakdowns of the most technologically important thin-film elements. Therefore, recognition of phenomena that are mainly responsible for stress in thin films is of much significance. Numerical simulations are very useful for the study of the behaviour of thin films at a microscopic level. It is more convenient and cheaper to examine wide ranges of parameter space and to optimize deposition conditions, such as deposition rate, substrate temperature, etc., using computer simulation rather than a protracted experimental search.

Recently, several authors proposed MD simulation and kinetic Monte Carlo simulation [1–7] to understand changes of the structure in growing films and their final properties. In particular, Paik *et al.* [1] used MD simulation to study the growth process on various orientations of a fcc substrate using Lennard–Jones potential. Their results showed that the best epitaxial film growth with the lowest numbers of lattice defects takes place along [100] and [111] directions. Guan *et al.* [2] found several parameters, which affect the type of the film growth. The deposition of Ag on Cu (100) at a high temperature causes the hexagonal close-packed structure to disappear at a low coverage.

Many of the above quoted publications concentrated on the modelling the real systems. The results of MD simulation of films of Co on Cu (001) [4] and Ni on Cu (001) [5] showed that these films exhibit a pseudomorphic growth. Moreover, it was also demonstrated that numerous parameters can affect the properties of

1 the films. In particular, for the systems containing the same kind of atoms [6, 7],
2
3 the topology and the roughness of the adsorbed layers may be quite different. For
4
5 example, the deposition rate, the substrate temperature and the incident angle can
6
7 drastically affect the morphology of deposited layers.
8
9

10 The papers cited above were focused on study of influence of the simulation
11
12 parameters on the morphology of growing films. Dong *et al.* [8] investigated the
13
14 dependence of the crystal lattice defects on the stress relaxation process, but
15
16 only for two-dimensional system. Several authors employed molecular dynamics
17
18 simulation to understand behaviour of stress in films [9, 10]. In particular, Zhang
19
20 *et al.* [9] used this technique to study the stress generation mechanism in thin film
21
22 grown by ion-beam deposition, whereas Kalyanasundaram *et al.* [10] presented
23
24 results of stress evolution during ion bombardment in silicon.
25
26

27
28 There have been reported experiments of thin film deposition that show growth
29
30 by Frank van der Merwe, Stranski-Krastanov, and Volmer-Weber mode. In the
31
32 Frank van der Merwe growth mode a crystal layer tends to be completed before
33
34 a new layer is started above and this mode is also called layer by layer growth.
35
36 In an opposite situation, i.e. in the Volmer-Weber growth mode the second
37
38 overlayer growth begins before the first monolayer is completed, producing a
39
40 three-dimensional islands. The Stranski-Krastanov case is an intermediate between
41
42 the Frank van der Merwe and the Volmer-Weber mode. The deposition process
43
44 near equilibrium state leads to layer by layer growth mode. Usually, experimental
45
46 measurements show three-dimensional growth. It should be stressed, however, that
47
48 the application of the Lennard-Jones potential in simulations always leads to the
49
50 Volmer-Weber growth mode [2].
51
52
53

54 In order to investigate the substrate influence on deposited layers that are built of
55
56 atoms of the same kind we performed a series MD simulations. The stress evolution
57
58
59
60

1 during the film growth is directly connected with the structure changes of the film.
2
3 The aim of our simulations was not to reproduce the behaviour of a particular
4 material, but rather to gain the knowledge about the film growth mechanism
5 on the atomic level and to predict the film properties. To do that we carried
6 out a three-dimensional molecular dynamics simulation of a thin film deposition
7 onto initially flat surface. In our simulations we have assumed that the atoms
8 interact via simple Lennard–Jones potential. This type of interatomic potential
9 provides a reasonable basis for modelling solids. First, we study the growth mode
10 and morphology of obtained thin films. Then, we examine the stress evolution in
11 film during deposition. A comparison of the present simulation results with those
12 obtained using more refined potentials would be very instructive and will be the
13 subject of future studies.
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29

30 2 Simulation model

31
32
33 The algorithm of three-dimensional MD simulations used in this work was described
34 by Allen and Tildesley [11]. Specifically, the trajectories of each atom were obtained
35 by integrating Newton's equation of motion and the integration was performed in
36 a step-wise manner over finite time steps by using a fifth-order predictor-corrector
37 method. The interaction between atoms was assumed to be pairwise additive and
38 the pair potential was represented by a truncated (12,6) Lennard Jones (LJ)
39 potential
40
41
42
43
44
45
46
47
48

$$49 \quad U(r) = \begin{cases} 4\varepsilon[(\sigma/r)^{12} - (\sigma/r)^6] & r \leq r_{max} \\ 0 & r > r_{max} \end{cases}, \quad (1)$$

50
51
52
53

54 where σ is the distance between the particles for which the potential is equal to 0, ε
55 is the strength of the interaction, and r_{max} is the cut-off distance, that is assumed
56 to be 3.5σ .
57
58
59
60

1 The simulations were carried out in a rectangular box of the dimensions
2
3 $L_x \times L_y \times L_z$ and periodic boundary conditions were applied in the x and y
4
5 directions. At the bottom of the box an unmovable solid wall was placed as a
6
7 substrate. This wall was assumed to be the (100) plane of a fcc regular crystal
8
9 characterized by the unit vectors a_1 and a_2 of the same length $|a_1| = |a_2| = a$.
10
11 Throughout the paper all the distances are expressed in units of a , and the energy
12
13 parameter of the potential (1), ε is the unit of energy. To prevent the atoms from
14
15 leaving the simulation box, a reflecting wall was set at its top.
16
17

18 The source that creates particles in the system was located at a sufficient
19
20 distance away from the bottom surface. This distance was equal to 45 in our
21
22 case. The particles were created at random (x, y) positions and initially lunched
23
24 perpendicular to the bottom surface.
25
26

27 The simulations were carried out for $L_x = L_y$ equal to 16, 20, 25, 30 and
28
29 for $L_z = 50$. The substrate crystals are formed by 15 atomic layers, i.e. for
30
31 $L_x = L_y = 16 \times 16$ the crystal contains 3840 atoms. We can distinguish two
32
33 regions in the simulated system. The region of a high concentration atoms (near
34
35 the bottom surface) corresponds to a solid film. However, the region with a low
36
37 atomic concentration corresponds to a vapour. The simulation was divided into two
38
39 stages: deposition and equilibration. The deposition process consist in repeating
40
41 sequence of creating a single atom, and equilibrating at a selected temperature.
42
43
44 Finally, the obtained system was equilibrated.
45
46

47 The interaction of a fluid atom with the surface was calculated by summing up
48
49 the LJ potentials
50
51

$$52 U_{gs}(r) = \begin{cases} 4\varepsilon_{gs}[(\sigma_{gs}/r)^{12} - (\sigma_{gs}/r)^6] & r \leq r_{gs,max} \\ 0 & r > r_{gs,max} \end{cases}, \quad (2)$$

53
54
55
56
57

58 over all the atoms of the wall. The cut-off distance, $r_{gs,max}$ was again equal to
59
60

3.5 σ_{gs} . We assumed that the size of the atoms is equal to $\sigma^* = \sigma_{gs}^* = 1.0$, and that $\varepsilon_{gs}^* = \varepsilon^* = 1.0$.

The reduced time was defined as usual [11], $t_0 = (m\sigma^2/\varepsilon)^{1/2}$, where m is the mass of the atom. The time step used to solve Newton's equations of motion was $\Delta t = 0.005t_0$. Hereafter the time is expressed as a number of the time steps. The temperature during the simulation was kept constant by periodical velocity rescaling. The method of simple velocity rescaling allows to keep the average temperature at required level. In our algorithm of simulation we rescaling velocity every 5-10 time steps. The observables of interest are dependent on the averages and this algorithm can be safely used [12]. The reduced temperature is defined as $T^* = k_B T/\varepsilon$, where k_B is the Boltzmann constant and T is the temperature in Kelvin. The deposition rate of atoms is expressed as a ratio of the number of deposited atoms per number of time steps. The lower value of this ratio corresponds to the lower value of real deposited rate. The energy of deposition was always equal to $E_k \approx 18eV$. This value corresponds to kinetic energy of a Cu atoms. One of the most suitable experimental methods for this purpose is physical vapour deposition.

Usually, the stress definition that considers the stress as the force acting on the face area is not suitable for atomic systems. For such systems the stress is determined by position of atoms resulting from interatomic potential. One of commonly used definition of the stress for atomic system is the virial stress, which is results from a generalization of the virial theorem of Clausius [13] for the gas pressure. According to this definition, the average stress tensor (S) over an effective volume is a sum of the contribution from all the atoms in the domain of the volume V .

$$S = \frac{1}{V} \sum_i^N \left(m_i v_i \otimes v_i + \frac{1}{2} \sum_{j \neq i} r_{ij} \otimes f_{ij} \right), \quad (3)$$

1 where m_i is the mass, v_i is the velocity of the atom i , $r_{ij} = r_i - r_j$ is the spatial
2
3 vector between atoms i and j , N is the total number atoms in the domain, and \otimes
4
5 denotes the tensor product of two vectors. The interatomic force f_{ij} applied on the
6
7 particle i by the particle j is
8
9

$$10 \quad f_{ij} = \frac{\partial U(r_{ij})}{\partial r_{ij}}, \quad (4)$$

11
12
13
14
15
16 The sign convention adopted here for the force such that it is positive for attraction
17
18 and negative for repulsion. Accordingly, a positive stress indicates expansion,
19
20 whereas a negative stress indicates compression.
21
22

23 The stress definition includes two parts. The first part stems from the kinetic
24
25 energy of the atoms, while the second part comes from interatomic forces. For
26
27 solids, the kinetic energy term is usually small compared to the interatomic force
28
29 term and is ignored. The stress is a (3×3) tensor, which can be represented in the
30
31 diagonal form:
32
33

$$34 \quad \bar{S} \equiv \begin{pmatrix} S_{xx} & 0 & 0 \\ 0 & S_{yy} & 0 \\ 0 & 0 & S_{zz} \end{pmatrix}, \quad (5)$$

35
36
37
38
39
40
41
42
43 where S_{xx} , S_{yy} and S_{zz} are stresses in the x , y and z directions. The film stress is
44
45 calculated when the system was equilibrated after each atom deposition.
46
47

48 The atoms are randomly deposited on the growing surface and each deposition
49
50 increases the film thickness. To determine the roughness of the growing surface
51
52 we calculated the interfacial width $W(t)$ from the simulation data. The width is
53
54 defined as:
55
56
57

$$58 \quad W(t) = [\langle h^2(t) \rangle - \langle h(t) \rangle^2]^{1/2}, \quad (6)$$

1 where
2
3

$$4 \quad h(t) = \frac{1}{L_x \times L_y} \sum_{\tau} h(\tau, t), \quad (7)$$

5
6
7

8 $h(\tau, t)$ is the thickness of the film at site $\tau = (x, y)$ and t is the time.
9
10

11 12 13 **3 Results and Discussion** 14

15
16 We have performed a series of MD simulations of the growing films on the solid
17 surfaces. Both, the surface and the gas atoms are of the same kind. It means that
18 the all the parameters of the interaction potentials are the same for all the atoms in
19 the system. In different simulation runs the temperature T^* , the rate of deposition
20 V , and the size of simulation cell was changed. However, the initial kinetic energy
21 of arriving atoms was kept constant and equal to $18eV$.
22
23
24
25
26
27
28

29
30 At the beginning of a single run, we simulated the growth of the film at
31 the selected temperature and the rate of deposition. Next, the obtained system
32 was equilibrated at the same temperature. During these two simulation steps
33 we calculated the thermodynamic and the dynamical data. **The averages of the**
34 **interesting quantities were accumulated after each 50 – 100 time steps. The number**
35 **of steps used for the equilibration ranged from 10^4 to 10^6 .**
36
37
38
39
40
41
42

43
44 Figure 1 shows an example of the typical configurations obtained during the
45 simulation at the temperature $T^* = 0.5$ and for the deposition rate equal to 1/100
46 (i.e. 1 atom was created after each 100 time steps). The curve of the total energy
47 shown in figure 2 exhibits a jump at the temperature of about $T_m^* = 0.68$. At this
48 temperature the film starts to melt [14]. The heat capacity curve, given in the inset
49 to figure 2, confirms this behaviour. Moreover, for different rates of deposition the
50 melting temperature was almost the same.
51
52
53
54
55
56
57

58
59 In the case of thin layer deposition it is very important to know what mechanism
60

1 governs the growth process. As we have already mentioned, there are three modes of
2 growth that depend on atom mobility on the surfaces. The films often grow with the
3 Volmer-Weber mode in a fast deposition process. The results of the film growth
4 obtained for $V = 1/20$ at four different temperatures are presented in figure 3,
5 where we plotted the number of atoms in each layer as functions of simulation time
6 for the first four layers. Note that in this case the system size was $16 \times 16 \times 50$,
7 so the full coverage of any layer corresponded to 256 deposited atoms. We see that
8 before completely filling the first layer, the second and next higher layers start to
9 be filled. At high temperature, $T^* = 1.0$, considerable fluctuation in the particle
10 number density per layer appear and the growth rate drops substantially due to
11 lower sticking ratio. From the results presented here it arises that the film grows
12 according to the Volmer-Weber mode.

13 We have also calculated roughness that appears during the deposition and the
14 equilibration. Typical shape of the curves obtained at the deposition stage is given
15 in figure 4. The curves plotted here were obtained from interpolation of original
16 data. They seem to confirm the mechanism of film growth according to the Volmer-
17 Weber mode. The roughness in figure 4 attains a maximum value for the coverage
18 equal about two monolayers (with 256 atoms per layer). Moreover, the position of
19 roughness maximum is almost independent on the simulation temperature. Next,
20 the roughness becomes smaller and starts rising as the result of an increasing film
21 thickness. Above the coverage equal to eight monolayers the surface roughness
22 increases linearly. The final value of roughness at the end of the deposition is
23 larger at higher temperature. This situation does not change after equilibration
24 of the systems. The curves of roughness possess the minimum value for the higher
25 coverage with decreasing the temperature. The diffusion ability of the growing
26 surface atoms increases with increase in temperature. In higher temperature the

1 adsorbed atoms faster fill up the inner voids of the film.

2
3 Figure 5 exhibits relationship between the roughness created during the
4 deposition and the system size at the temperature equal to 0.4. The maximum of the
5 roughness increases with an increase of the system size for all systems under study,
6 in accordance with the scaling theory [15]. Simultaneously, for larger systems the
7 maximum of the roughness shifts slightly towards lower thickness of the adsorbed
8 layer.
9

10 In figure 6 we present the evolution of the mean biaxial stress, $S_{xy} = (S_{xx} +$
11 $S_{yy})/2$, versus the number of adsorbed layers for different system sizes. The
12 rate of deposition equals 1/100 and the temperature is $T^* = 0.4$. The value
13 of the maximum stress falls down with the increasing system size. The position
14 of the stress maximum corresponds to coverage of about two monolayers and
15 is slightly shifted towards higher film thickness for larger systems. In order to
16 explain the observed stress evolution we performed calculations of the mean biaxial
17 stress for each deposited layer separately. A typical result for separate monolayer
18 contributions is given in figure 7. We observe that the shape of the function
19 describing the stress versus the coverage in the first monolayer agrees with the
20 shape of the curve for the mean biaxial stress obtained for all the deposited atoms
21 (figure 6). Moreover, the stress in the next monolayers exhibits only little changes
22 towards the compressive stress. These changes are much smaller than the changes
23 of the stress in the first monolayer. Thus, the first monolayer yields the most
24 important contribution to the mean biaxial stress of the deposited film.
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49

50 Figure 8 displays the biaxial stress S_{xy} and the normal stress S_{zz} versus
51 the number of deposited atoms, obtained for the growth rate equal to $V =$
52 1/100 at different temperatures. The shape and the behaviour of the curves are
53 quite different at different temperatures. Our simulations also indicated that the
54
55
56
57
58
59
60

1 behaviour of stress strongly depends on the deposition rate. Moreover, the change
2
3 of interatomic distances or adsorption of atoms from the gas may also lead to
4
5 changes of the stress. However, we should stress again that the appearance of the
6
7 stress maximum at the coverage equal to about two layers is characteristic.
8
9

10 The maximum value of the biaxial stress strongly depends on the temperature
11
12 and decreases with increasing the temperature of the substrate. Such evolution of
13
14 the biaxial stress is often linked with a change in the grain structure of thin films.
15
16 In contrast to the biaxial stress, the stress in normal direction is less sensitive
17
18 to the number of deposited atoms and its value is smaller when compared with
19
20 the value of biaxial stress. In this case, we do not observe stress in the normal
21
22 direction at the first stage. When the biaxial stress achieves its maximum value we
23
24 also observe an increase in the normal stress. After that, the value of the normal
25
26 stress becomes smaller and tends to zero. At a high temperature the majority of
27
28 individual atoms is on the surface, but at lower temperature there are individual
29
30 atoms in the space between grains. That difference explains the faster changes in
31
32 biaxial stress in compressive direction for $T^* = 0.4$.
33
34
35
36
37
38
39

40 **4 Conclusion**

41
42 The results of molecular dynamics simulation of the film growth, morphology and
43
44 stress evolution during atoms deposition have been presented. The simulations
45
46 show that the films grow with the Volmer-Weber mode and a typical behaviour
47
48 of the stress for this kind of films has been observed. The main contribution to
49
50 the stress in films comes from the first monolayer. This is a consequence of the
51
52 strong affect of the substrate. The effect of the substrate decreases with increasing
53
54 film thickness. With the increasing system temperature the value of the maximum
55
56 stress decreases. The roughness exhibits a maximum value at the coverage equal
57
58
59
60

1 two monolayers. The final value of the roughness at the end of the deposition is
2
3 larger at higher temperature.
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

For Peer Review Only

References

- [1] S.M. Paik, S. Das Sarma, *Phys. Rev. B*, **39**, 1224 (1989).
- [2] P.Guan, D.R. Mckenzie, B.A. Pailthorpe, *J. Phys. Conds. Matter*, **8**, 8753 (1996).
- [3] C.M. Gilmore, J.A. Sprague, *Phys. Rev. B*, **44**, 8951 (1991).
- [4] N. Levanov, V.S. Stepanyuk, W. Hergert, O.S. Trushin, K. Kokko, *Surf. Sci.*, **400**, 54 (1998).
- [5] J.C. Jiménez-Sáez, A.M.C. Pérez-Martín, M. Said-Ettaoussi, J.J. Jiménez-Rodríguez, *Nucl. Instr. and Meth. B*, **228**, 64 (2005).
- [6] L. Wang, P. Clancy, *Surf. Sci.*, **473**, 25 (2001).
- [7] P. Zhang, X. Zheng, S. Wu, J. Liu, D. He, *Vacuum*, **72**, 405 (2004).
- [8] L. Dong, J. Schnitker, R.W. Smith, D.J. Srolovitz, *J. Appl. Phys.*, **83**, 217 (1998).
- [9] S. Zhang, H.T. Johnson, G.J. Wagner, W.K. Liu, K.J. Hsia, *Acta Mater.*, **51**, 5211 (2003).
- [10] N. Kalyanasundaram, M.C. Moore, J.B. Freund, H.T. Johnson, *Acta Mater.*, **54**, 483 (2006).
- [11] M.P. Allen and D.J. Tildesley, *Computer Simulation of Liquids*, Clarendon Press, Oxford, (1987).
- [12] G. Bussi, D. Donadio, M. Parrinello, *J. Chem. Phys.* **126**, 14101, (2007).
- [13] R. Clausius, *Philos. Mag.*, **40**, 122, (1970).
- [14] J.Q. Broughton, G.H. Gilmer, *J. Chem. Phys.*, **79**, 5119 (1983).
- [15] A.L. Barabási, H.E. Stanlay, *Fractal Concepts in Surface Growth*, Cambridge Univ. Press, Cambridge, (1995).

Figure captions:

Fig.1: Three-dimensional configurations obtained from simulations at $T^* = 0.5$ with the deposition rate equal to $1/100$. The numbers of deposited atoms are: a) 100, b) 500, c) 1500, d) 3000. At the bottom there is the solid wall, above which the deposited film grows.

Fig.2: The total energy versus the reduced temperature at the different deposition rates. In the inset the plot of the heat capacity (C_v) vs. temperature is presented.

Fig. 3: The number of atoms in successive adatom layers (from left to right) as a function of molecular dynamics simulation time steps for different temperatures. The rate of deposition is equal to $1/20$.

Fig. 4: The interpolated roughness of the growing film as a function of the number of deposited atoms for different temperatures, given in the picture.

Fig. 5: The roughness of the growing film as a function of the number of deposited atoms for different system size. The rate of deposition is equal to $1/100$ and $T^* = 0.40$.

Fig. 6: The stress evolution in the growing film vs. the number of deposited atoms for selected temperatures. The deposition rate is equal to $1/100$. S_{xy} is the mean biaxial stress and S_{zz} is a normal stress.

Fig. 7: The dependence of the mean biaxial stress in selected layers on coverage. The rate of deposition is equal to $1/100$ and $T^* = 0.40$. The simulation cell is $20 \times 20 \times 50$.

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

Fig. 8: The mean biaxial stress evolution during simulation versus of the number deposited atoms for different system size. The rate of deposition is equal to 1/100 and $T^* = 0.40$.

For Peer Review Only

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

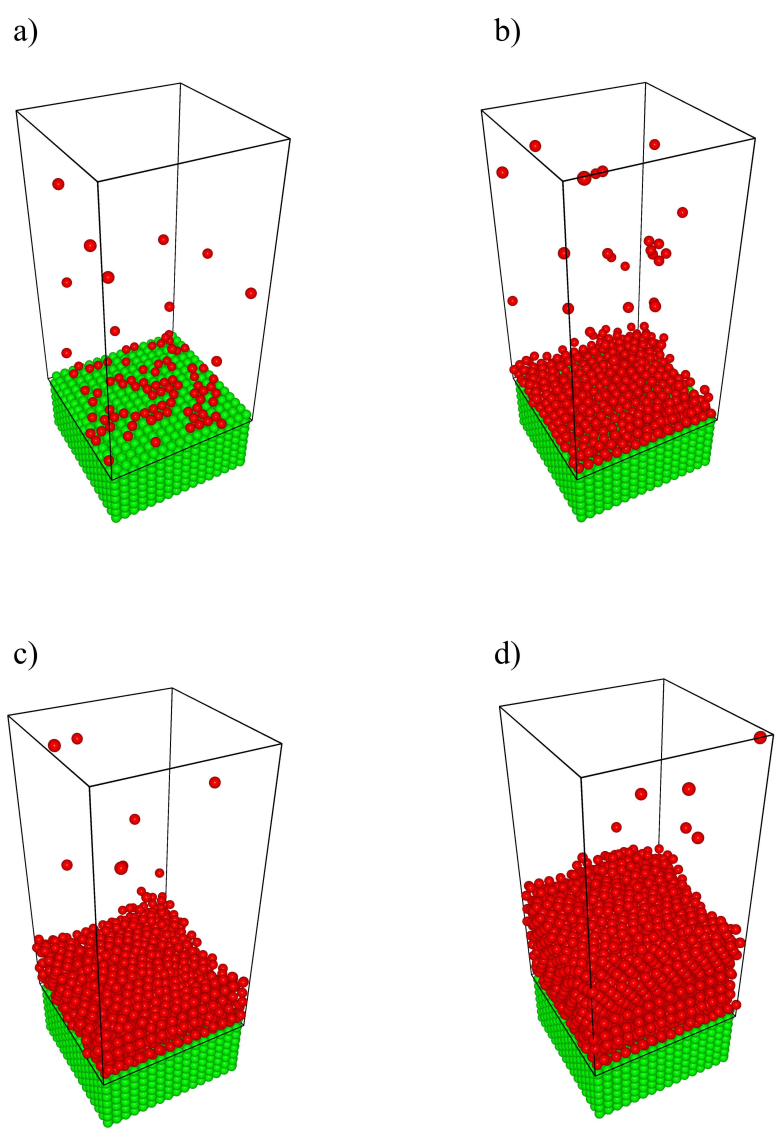


Fig. 1. T. Zientarski ...

ew Only

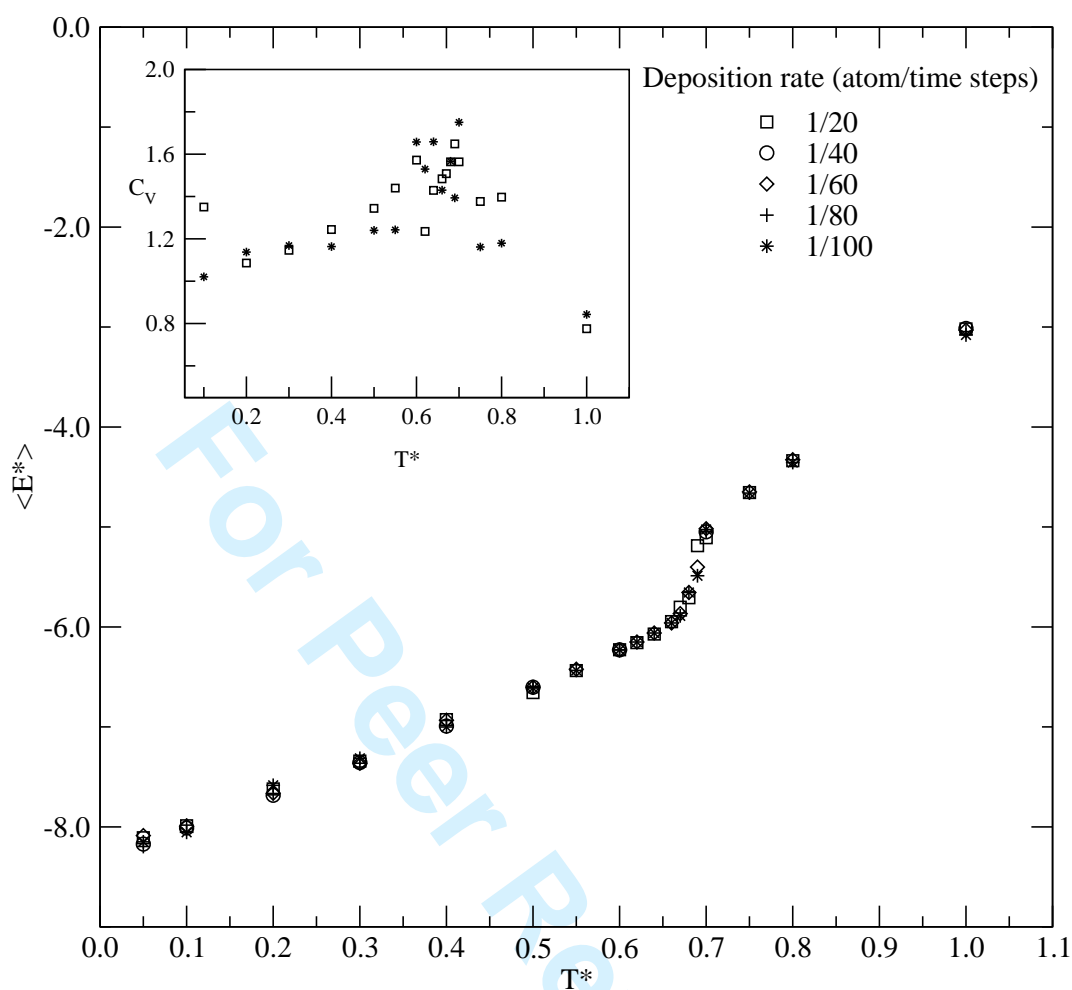


Fig. 2. T. Zientarski ...

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

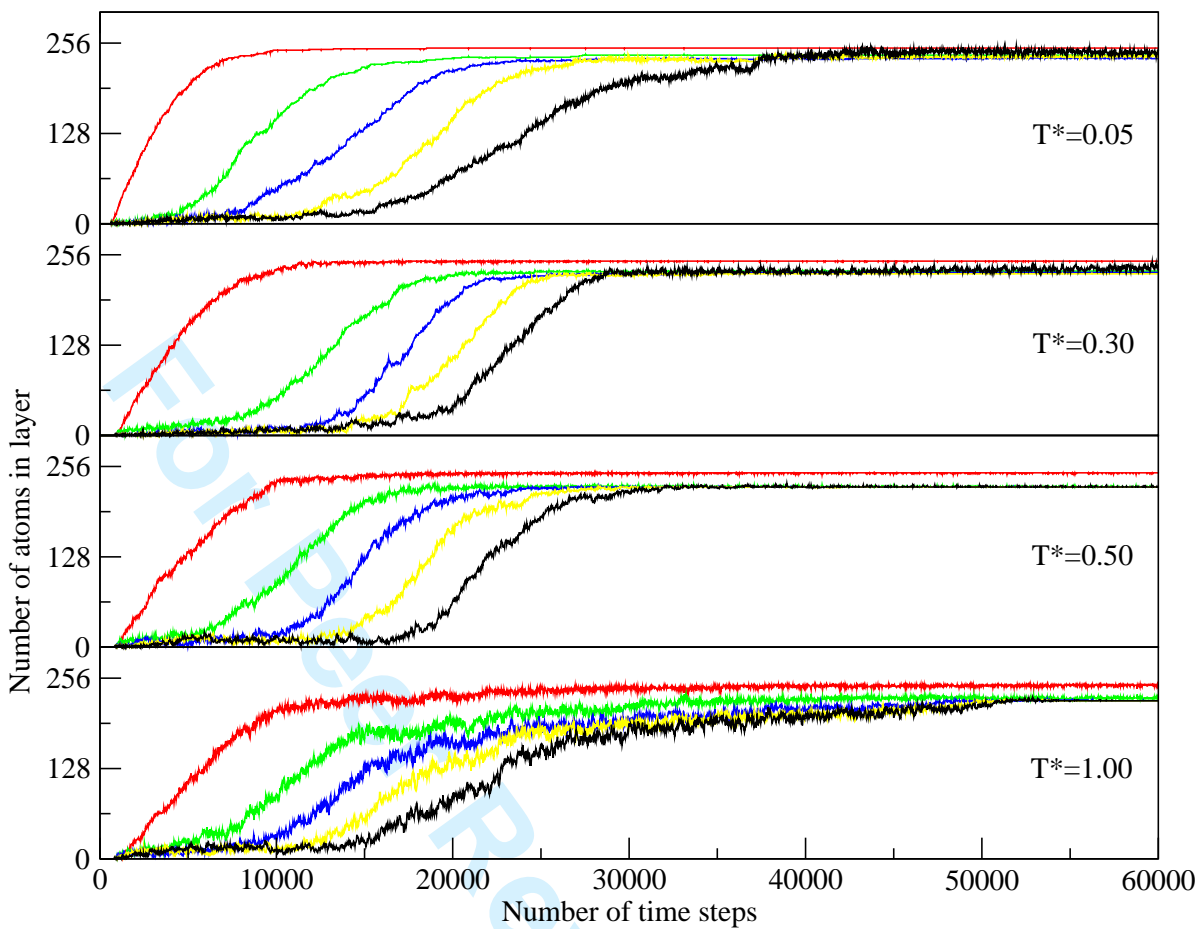


Fig. 3. T. Zientarski ...

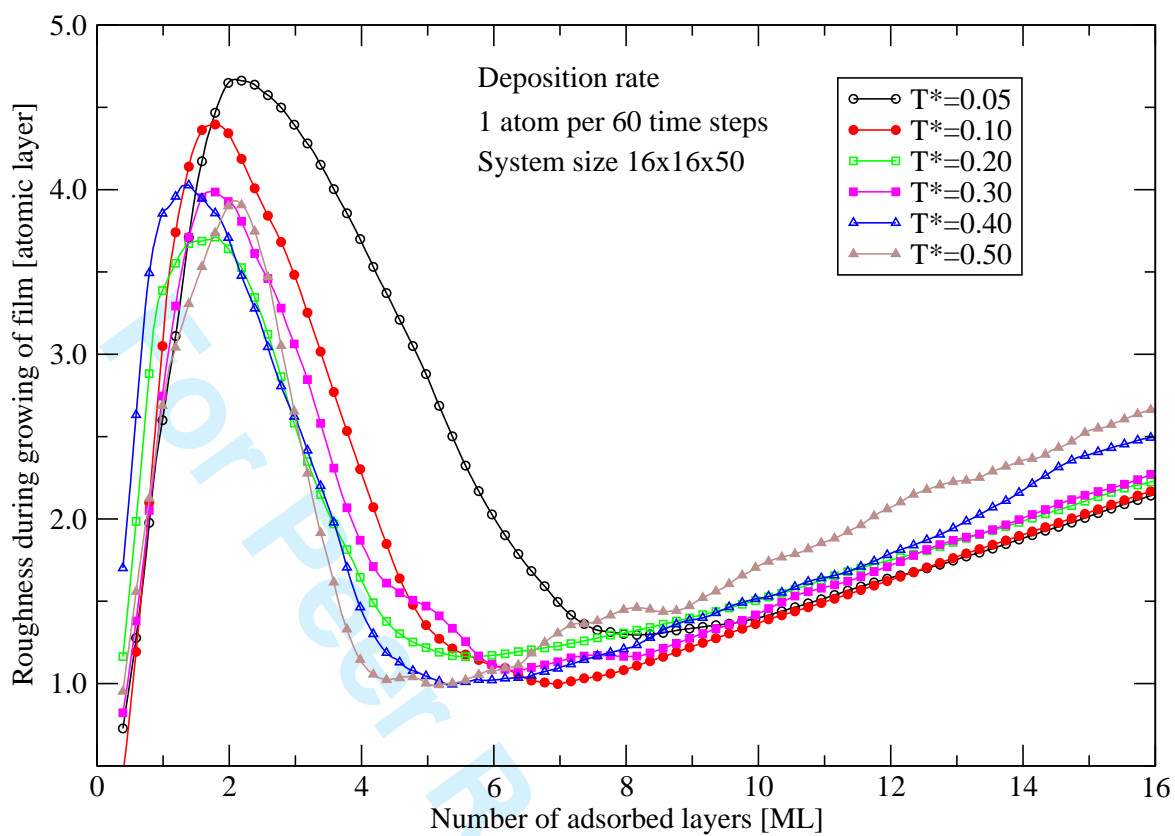


Fig. 4. T. Zientarski ...

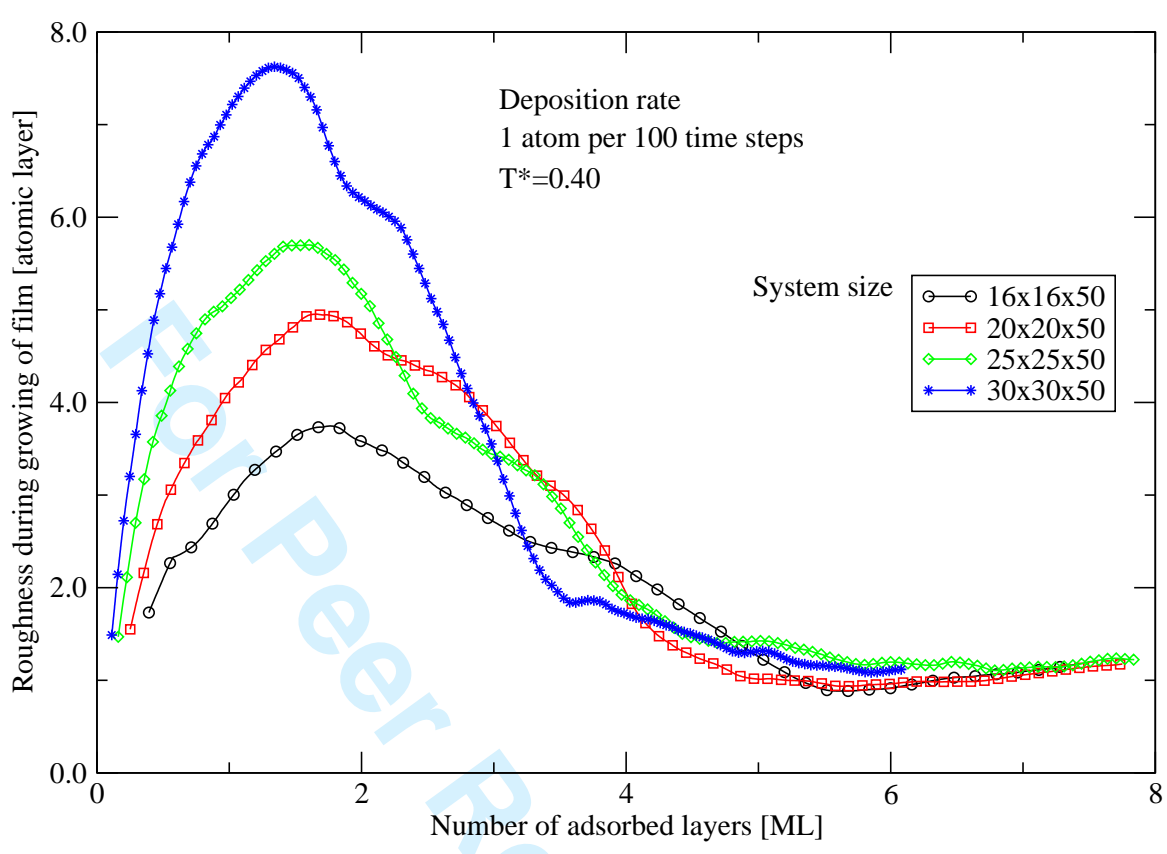


Fig. 5. T. Zientarski ...

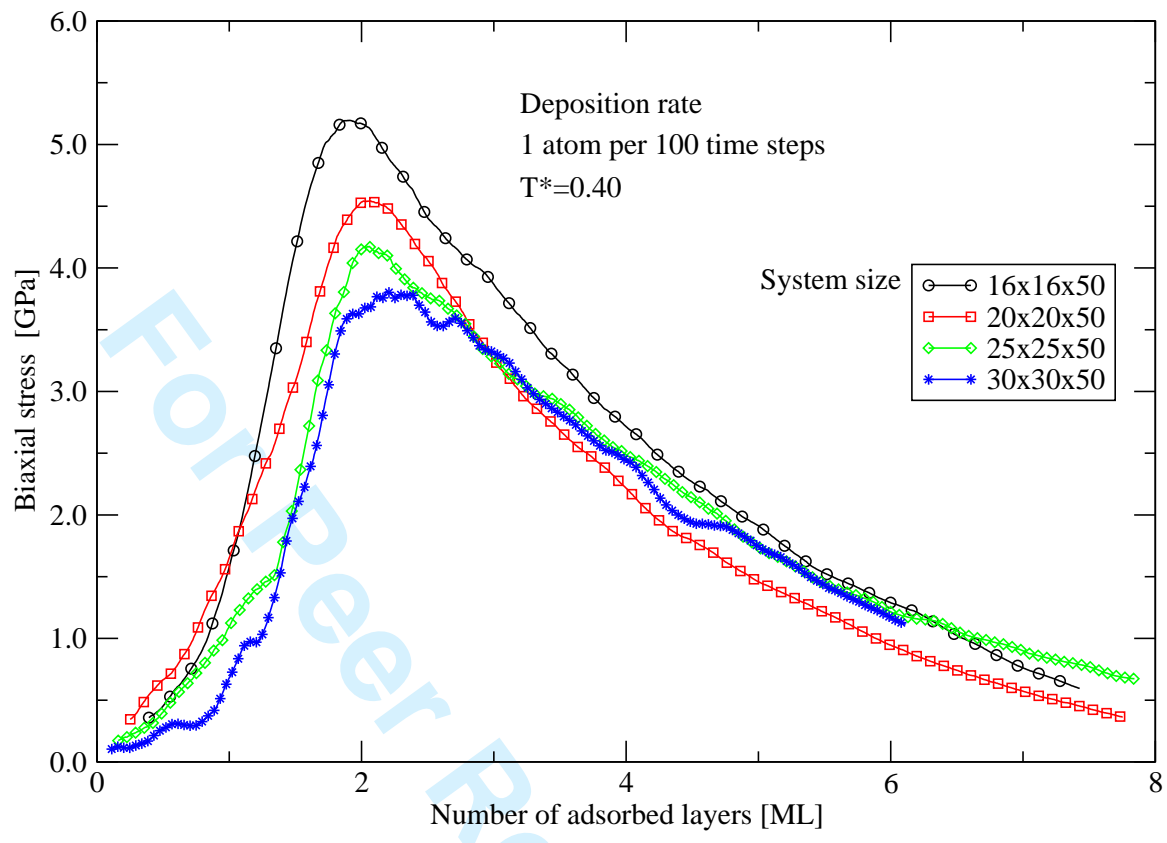


Fig. 6. T. Zientarski ...

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

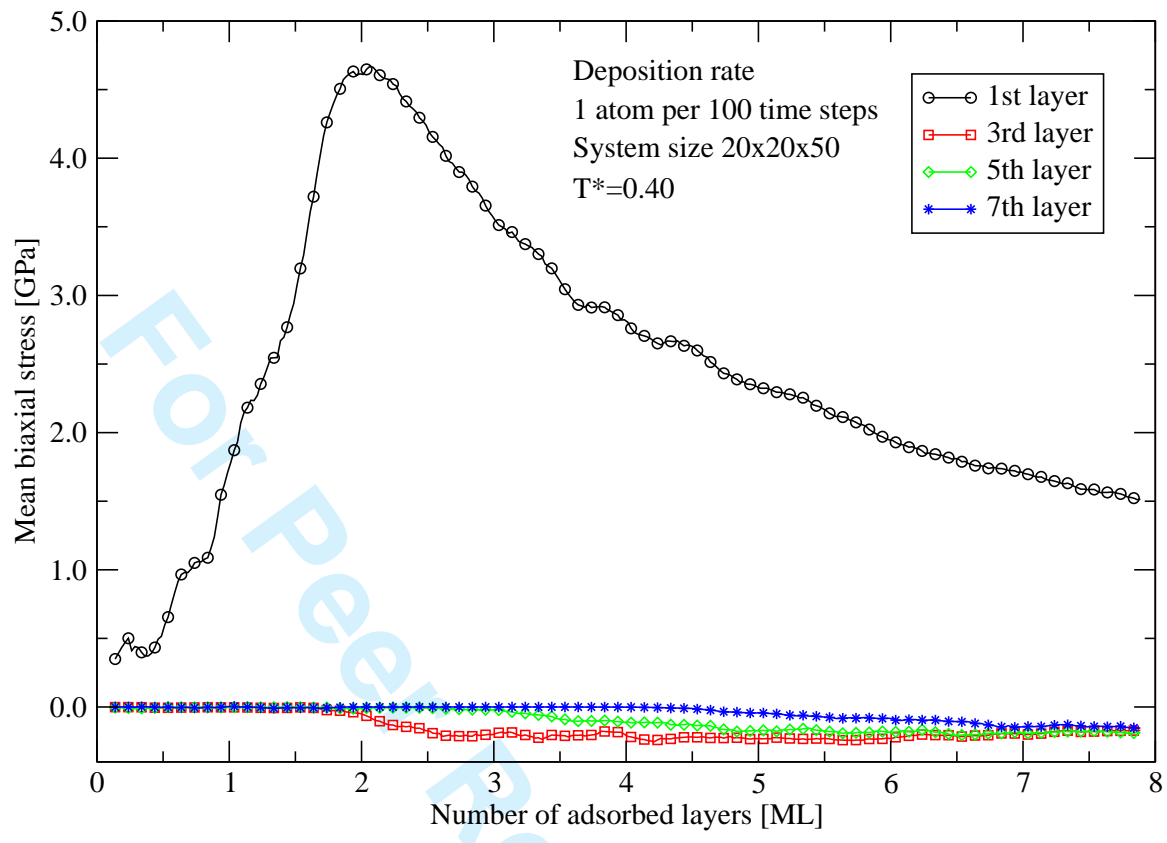


Fig. 7. T. Zientarski ...

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60

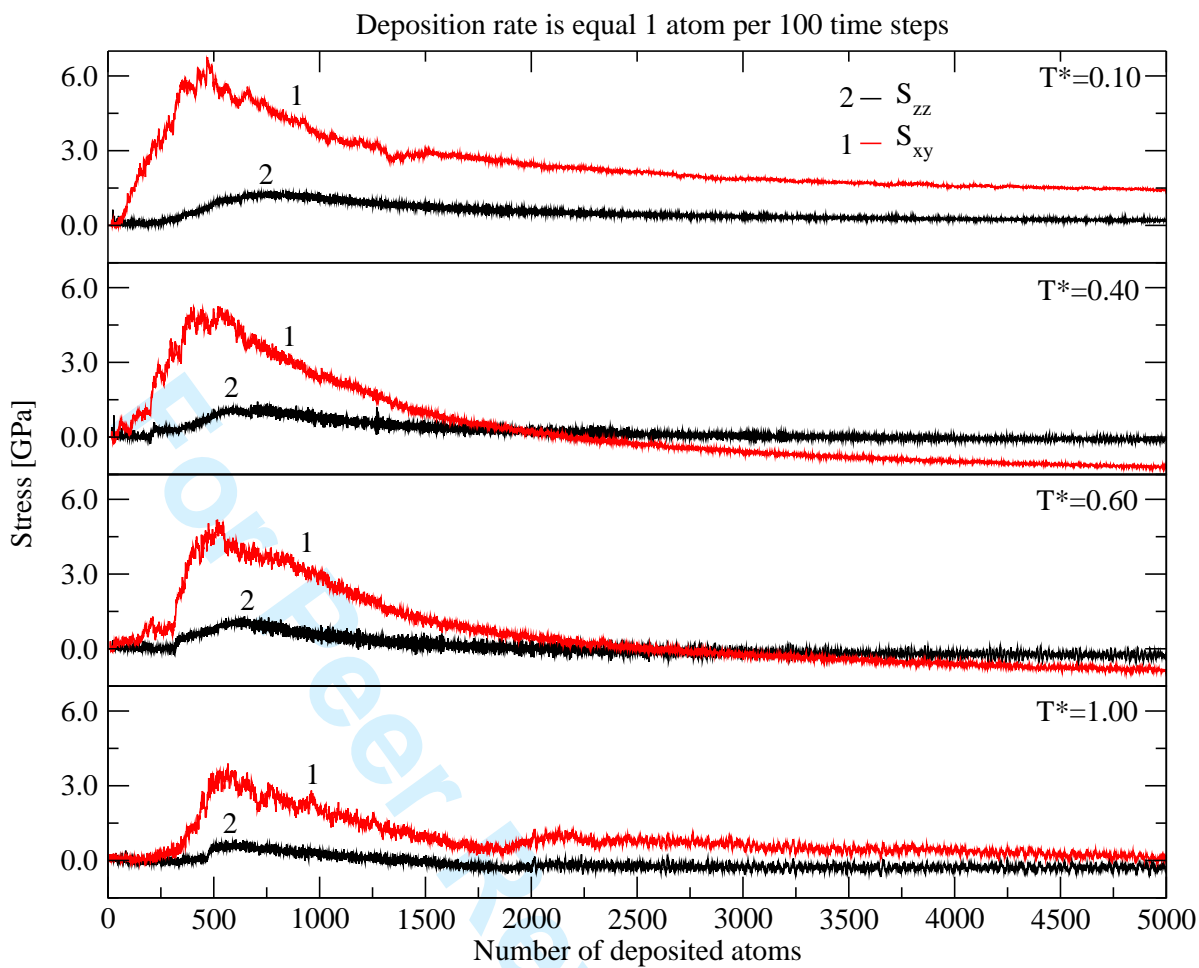
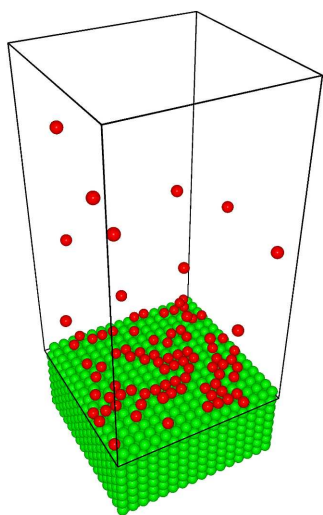
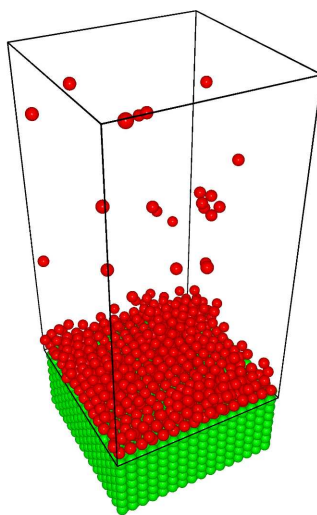


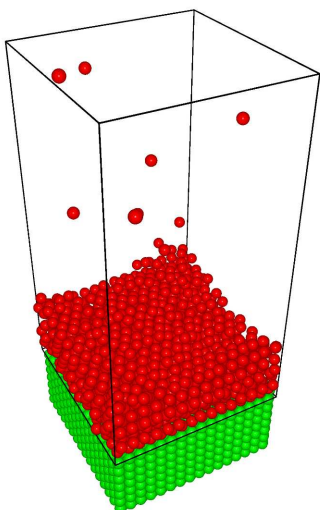
Fig. 8. T. Zientarski ...

1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49
50
51
52
53
54
55
56
57
58
59
60
a)

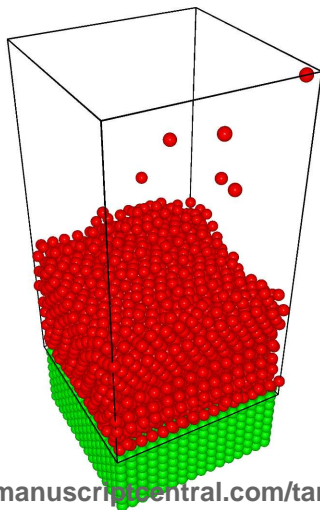
b)



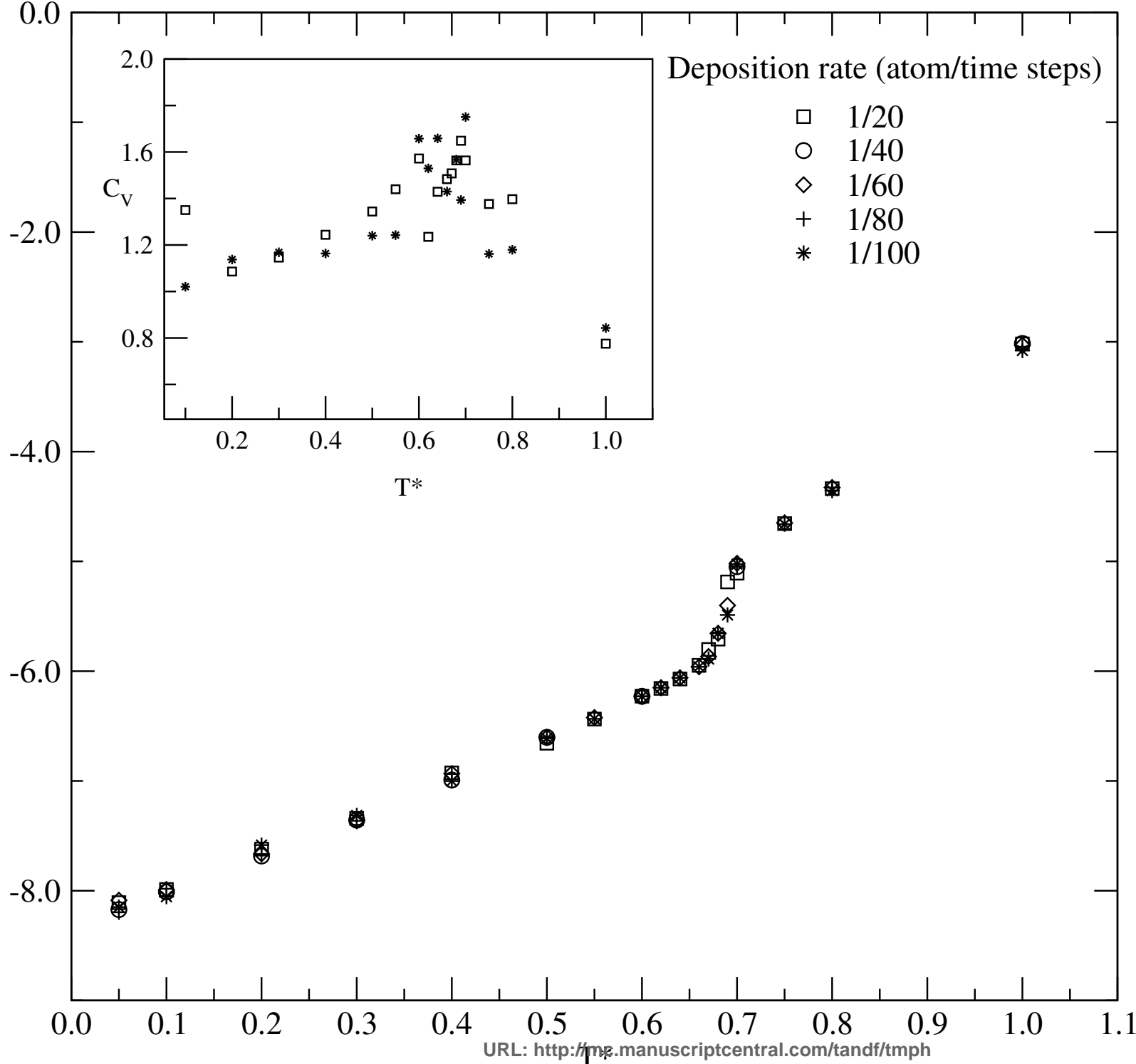
c)

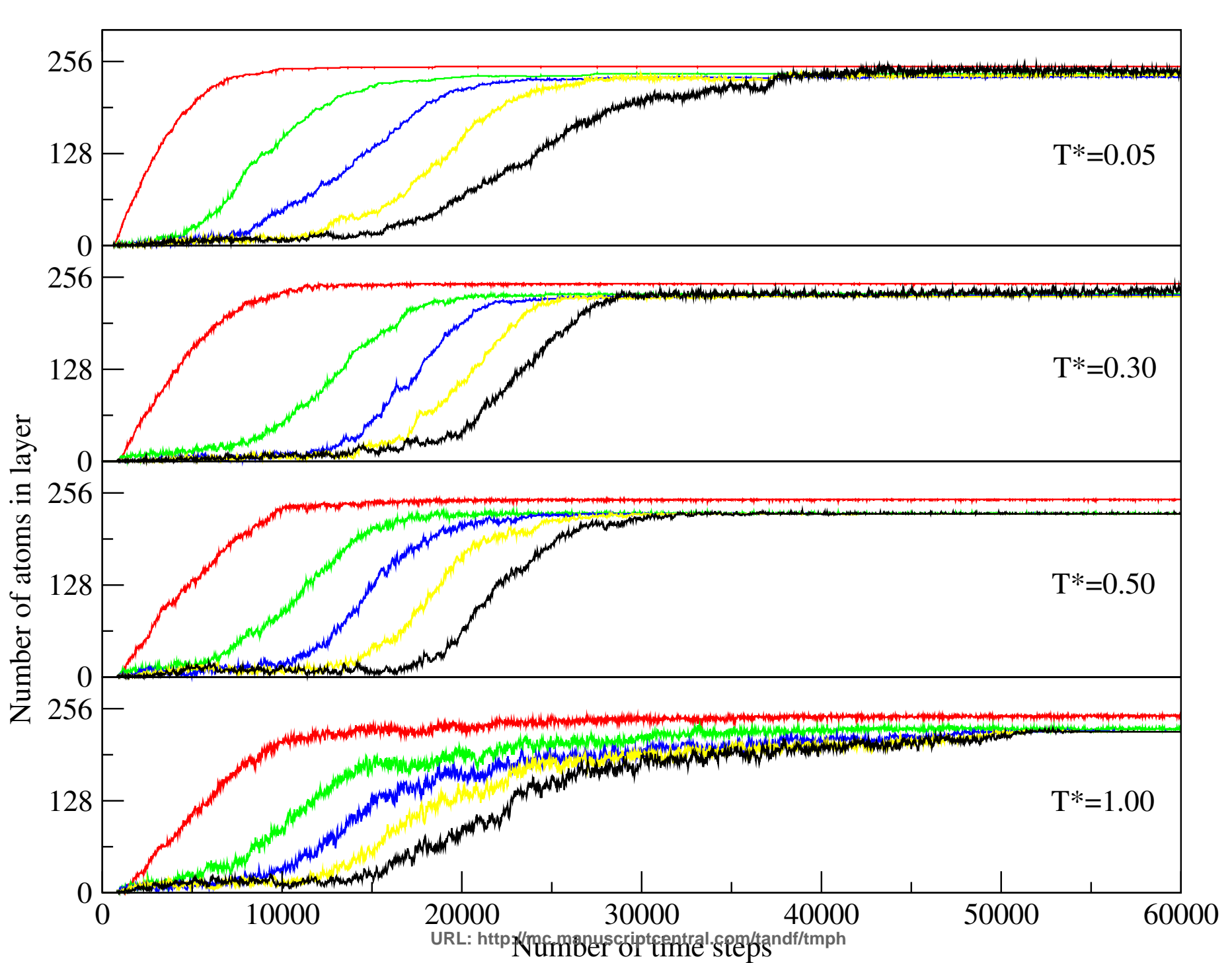


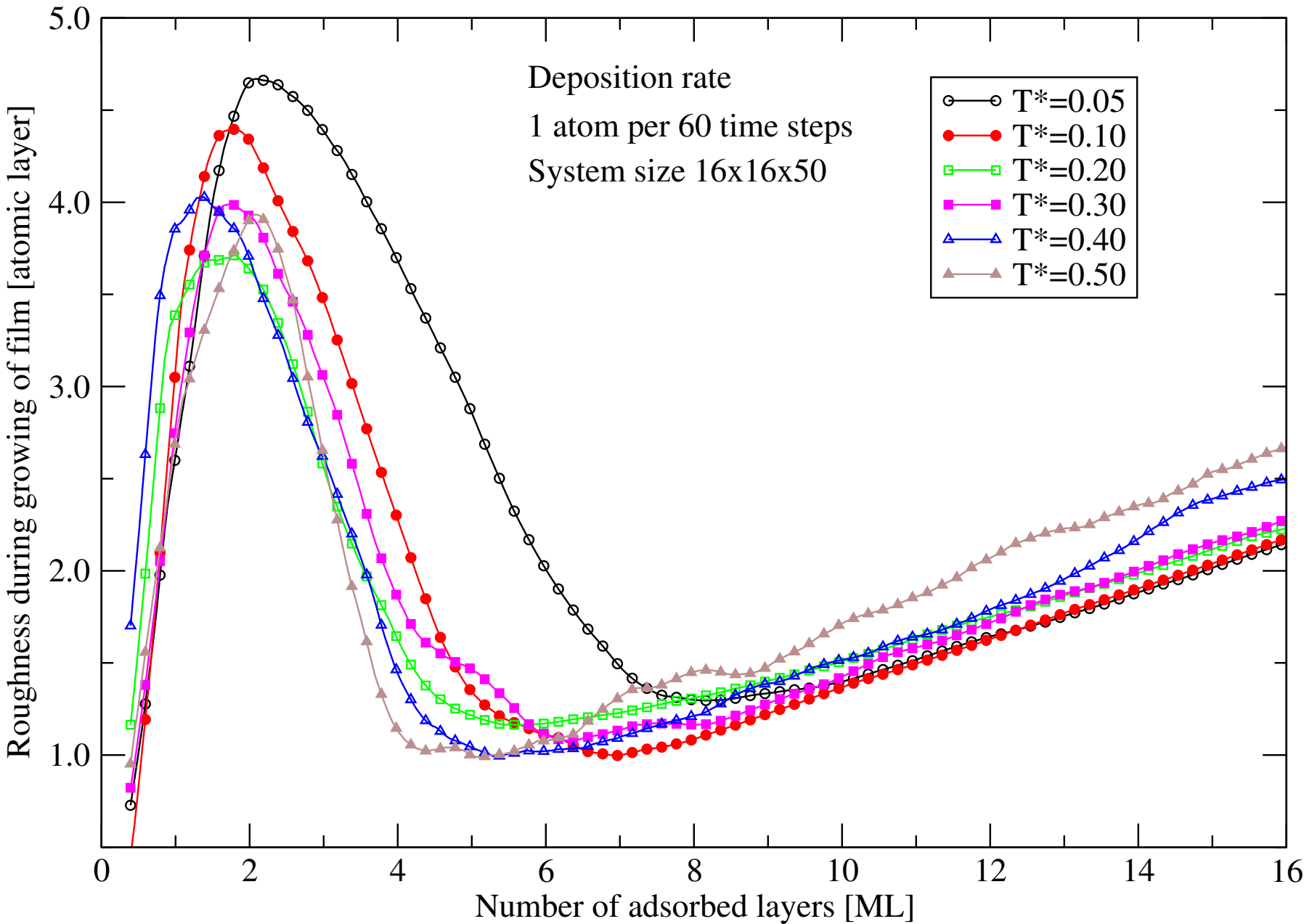
d)

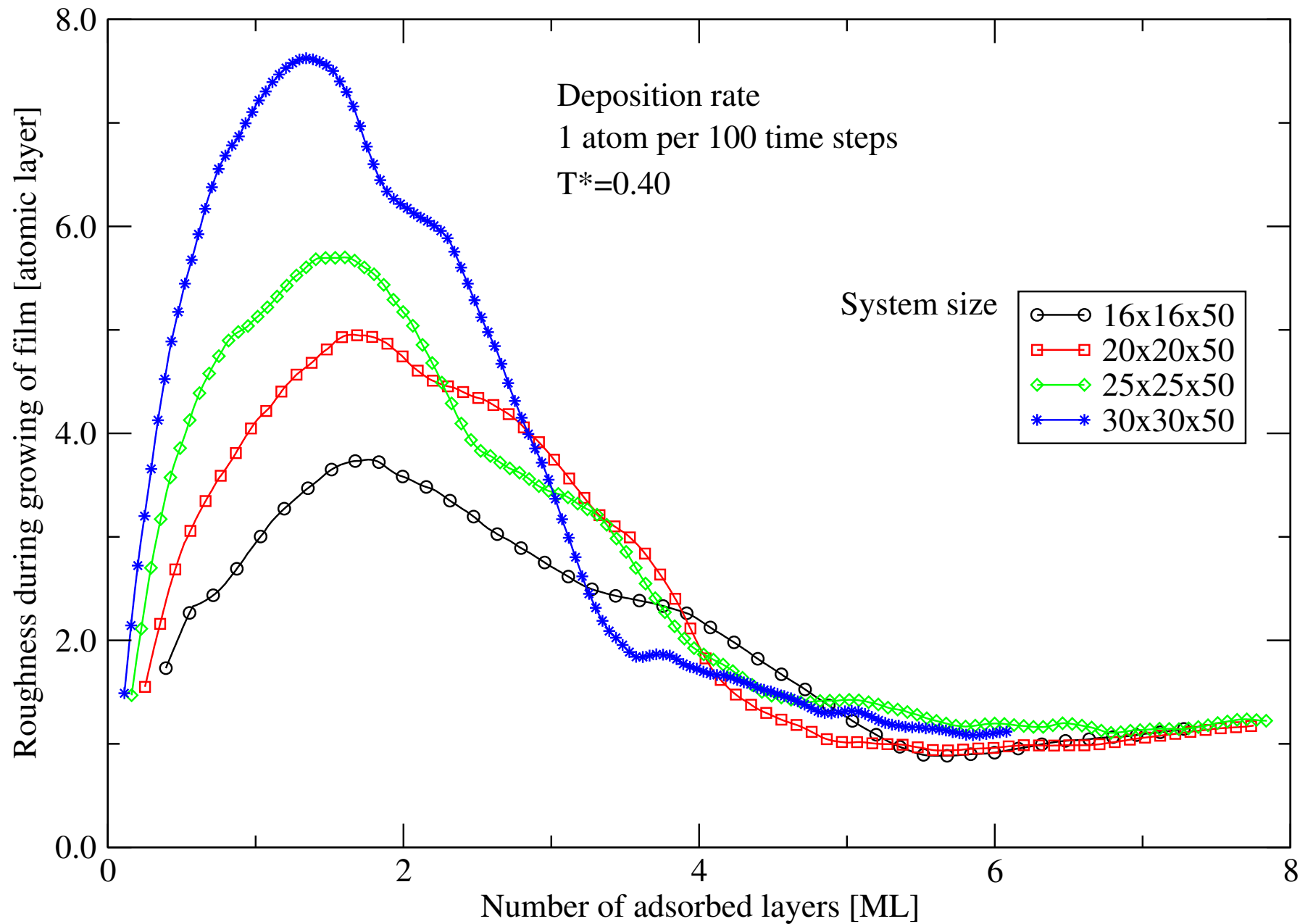


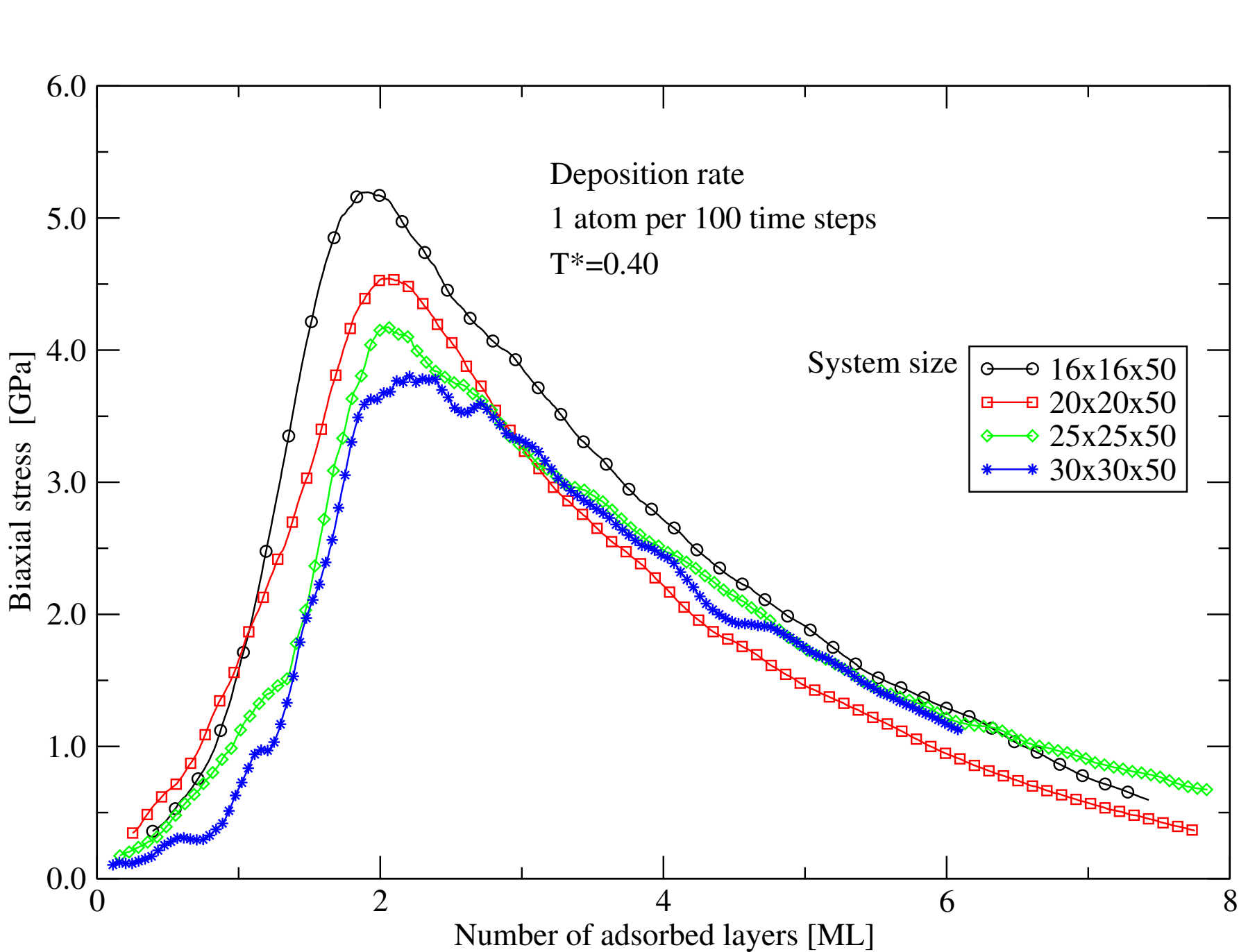
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
25
26
27
28
29
30
31
32
33
34
35
36
37
38
39
40
41
42
43
44
45
46
47
48
49

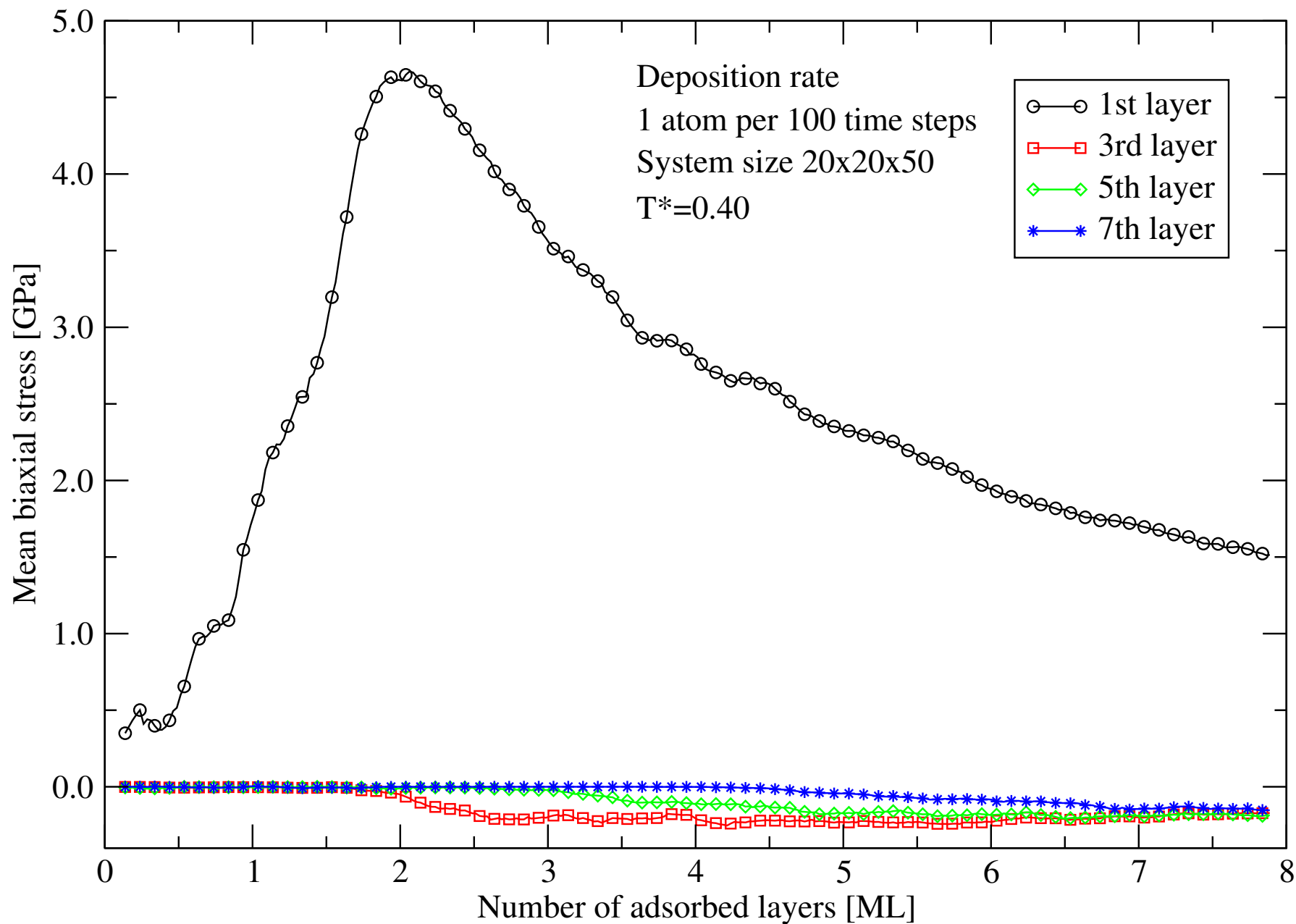












Deposition rate is equal 1 atom per 100 time steps

