DOI: https://doi.org/10.36094/sc.v89.2023.Simulation_Study_of_the_Scaling_Exponents.Das.393

ARTICLE

Sci. and Cult. 89 (11–12) : 393-399 (2023)

SIMULATION STUDY OF THE SCALING EXPONENTS FOR COMPETITIVE GROWTH BETWEEN BALLISTIC DEPOSITION AND RANDOM DEPOSITION WITH SURFACE RELAXATION IN 2+1 DIMENSIONS

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For distinct sets of values of the competitive growth parameter and the system size, rough surfaces were created by computer simulation for competitive growth between Random Deposition with Surface Relaxation and Ballistic Deposition. The evolution appeared with two regimes of time growth with two acutely different slopes and a saturation regime with zero slopes. The reliance of the scaling exponents and the fractional porosity on the competitive growth parameter and system size is reported. The scaling exponents are found to have some deviation from the relevant universality classes.

Introduction

Modern research in material science for the comprehension of many physical and chemical phenomena includes the morphological study of surface growth and interface evolution. A rough surface is developed either when a single type of particle is deposited using the same growing mechanism[1–4], or when a single type of particle is deposited using a variety of growing mechanisms[5,6], or by the deposition of two or more different kinds of particles[7,8] in the 1+1 dimensions. In the 2+1 dimensions, the same holds true.

Different growth models, such as random deposition (RD), ballistic deposition (BD), random deposition with surface relaxation (RDSR), solid-on-solid model (SOS), body-centered solid-on-solid model (BCSOS), competitive growth model (CG), and many others, are available depending on the growth mechanism. Since these models are based on simple stochastic growth principles that, aside from RD, adhere to closest neighbour interaction, they can successfully simulate surface growth.

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The interface width W and average height $\bar{h}$ are the defining parameters for surface roughness and film thickness. Consider a square plane of system size L comprising of $L \times L$ number of sites of deposition. If the site (i, j) has a height $h(i, j, t)$ at the time t, then the average height and interface width are measured using

$$\bar{h}(t) = \frac{1}{L^2}\sum_{i=1}^{L}\sum_{j=1}^{L} h(i, j, t) \tag{1}$$

$$W(L, t) = \sqrt{\frac{1}{L^2}\sum_{i=1}^{L}\sum_{j=1}^{L}\left[h(i, j, t) - \bar{h}(t)\right]^2} \tag{2}$$

When particles are deposited at random, there is no association between them, and the interface width keeps increasing over time. In surface correlation-based deposition models, interface width first rises with time and reaches saturation after a particular period of time, referred to as the critical time or the cross-over time (t_x).

As a result, two zones with distinct power laws and scaling exponents exist in the time-evolution of interface

width, separated by a critical time. The growth exponent represents dynamic growth over time, and the roughness exponent represents saturation behaviour. The Family-Vicsek scaling relation[2,3] best describes the overall progression of the rough surface as

$$W(L,t) \sim L^{\alpha} f\left(\frac{t}{L^{z}}\right) \tag{3}$$

where $z\left(=\alpha/\beta\right)$ is the dynamic exponent, $f(u) \sim u^{\beta}$ for $u \ll 1$ and $f(u) \sim$ constant for $u \gg 1$.

Uniquely defining the several universality classes of the growth process are the scaling exponents (α, β and z). The "Edwards-Wilkinson" (EW) universality class, also known as the linear universality class, represents surface correlation via lateral diffusion of the particles at the surface. The "Kardar-Parisi-Zhang" (KPZ) universality class, also known as the non-linear universality class, shows surface correlation with lateral sticking of the particles at the surface without diffusion. The RDSR and BD models fit, respectively, into the EW and KPZ universality classes. Following are expected scaling exponent values for various universality classes in the 2+1 dimensions: Table-1 lists the exponent values for these universality classes for 2+1 dimensions as compiled from various research publications[1].

Table-1: The scaling exponent values for different universality classes in 2+1 dimensions

Universality Class	α	β	z
RD	-	0.50	-
EW	-	-	2.00
KPZ	0.33	0.24	1.67

The grown media generated voids in the presence of the BD model. This leads to a porous medium whose porous capacity is estimated in terms of fractional porosity. It is defined as

$$\sigma = \frac{N_v}{N_v + N_p} \tag{4}$$

where N_v is the number of voids and N_p is the number of particles deposited.

There are numerous studies that have examined surface growth with similar particles that follow the same stochastic growth rule, similar particles that follow a different stochastic growth rule, or particles of various shapes and sizes that obey a particular growth mechanism with various physical parameters influencing the roughness of the surface growth.

In 2001, Horowitz and Albano, for instance, investigated the competitive growth between random and ballistic deposition and offered a new scaling for that growth[5,6]. Although the scaling exponents depended on system size, Rodrigues et al. derived scaling exponents for higher dimensions that were consistent with the KPZ universality class[9]. T. A. de Assis and colleagues investigated the uneven scaling in the surface growth process[10]. The aforementioned two groups[9,10], Mello[11], Rocca et al.[12], El-Nashara and group[13,14], and many others have reported on the relationship of the growth exponent on the system size L and the probability p of deposition under the BD model. Horowitz[5], Rocca et al.[12], Chame et al.[15], and El-Nashara et al.[14] reported a continuous transition from the lower particle interaction model to the higher for competitive growth model. Yu and Amar presented a roughening phase transition effect for scaling a surface through the BD model in 2002[16]. The values obtained from discrete microscopic models, $\alpha \approx 0.33 - 0.40$ and $\beta \approx 0.20 - 0.25$, respectively, are substantially larger than the values obtained from the numerical solution of the KPZ equation, which were $\alpha \approx 0.18$ and $\beta \approx 0.09 - 0.15$ for 2+1 dimensions[17,18]. For their simplified erosion model that accounts for both particle-particle and particle-environment interactions, Nath et al. reported a variation in scaling exponents in the 2+1 dimensions, but the overall scaling adheres to the KPZ universality class[19]. In 2017, Kartha researched the non-equilibrium growth of patchy particles with anisotropic interaction in 1+1 dimensions, and it was noted that surface roughness and aggregate porosity depend on the size of the patch[20]. Banerjee et al. (2013) investigated the competitive growth of RD and BD while taking into account the particle interaction force, and they discovered that the scaling exponent was dependent on the newly proposed sticking parameter[21]. Kolakowska and Novotny suggested a novel scaling in 2015, along with a variation of scaling exponents for competitive growth[22]. The potential adherence rule model with an additional adsorption barrier (PARMA) that Reis et al. suggested had a scaling exponent that was consistent with KPZ universality class[23]. Roman et al. developed a new ballistic deposition model in 2022 while taking the depositing site's memory into account[24]. For their model, they suggested a new scaling with roughness exponent $\alpha = 2$, growth exponent $\beta = 1.25$, and a new exponent $\gamma = 0.50$, resulting in $z = (\alpha + \gamma)/\beta = 2$. Gomes-Filho et al. provided an alternative formulation of the scaling exponents for the KPZ universality class in 2+1

dimensions, which was consistent with the outcomes of thin film experiments and accurate simulations[25]. In their work, Almeida et al. reported a novel KPZ universality class scaling[26]. The effect of scaling exponents on particle size was reported by Sharafedini et al. in 2015[27]. The scaling exponents' influence on correction strength was demonstrated by Hosseinabadi et al., and the scaling exponents were adjusted in light of the correction strength[28].

In light of this, the author reported the development of a surface in 2+1 dimensions via competitive growth between RDSR and BD in this work. Additionally, the author examined the variation of various parameters, including interface width, growth exponent, roughness exponent, dynamic exponent, critical times, and porosity. The fields of material science and thin-film growth will greatly benefit from this in-depth investigation.

The Model and Simulation

Through computer simulation, this work supports the scaling exponent values for CGM involving RDSR and BD in 2+1 dimensions. The competitive growth parameter p denotes the fraction of deposited particles that adhere to the RDSR mechanism. In other words, $p = 0$ implies pure BD deposition and $p = 1$ denotes pure RDSR deposition. The deposition scheme (RDSR or BD) and the deposition site (i, j) are randomly selected. According to the BD model, the depositing particle adheres to the NNN (next to the nearest neighbour) site with the highest height. According to the RDSR model, the depositing particle falls to the site of deposition and then diffuses to the closest neighbouring site with the lowest height, raising the diffusing site's height by a factor of one. The deposited particle adheres to the top of the deposition site when two or more of the nearest neighbouring sites have the same maximum or minimum height. The four nearest neighbours of the depositing site are considered for the study.

The deposition was made for different sets of values of the competitive growth parameter p(= 0.00, 0.25, 0.50, 0.75, 0.90, and 1.00) and the system size L(= 16, 32, 64, and 128). Initially, the heights of all the sites are set to zero. To make each site equally likely, the system size should be equal to the number of particles deposited per unit of time. After each unit of time, the height of the individual sites, the average height, and the interface width were recorded. For 8000 units of time, the deposition was sustained in order to reach a profound saturation regime. A 100-event ensemble average of the data was used for the graphical representation and associated calculations.

Fig. 1 depicts the deposition scheme in a 1+1 dimensional space.

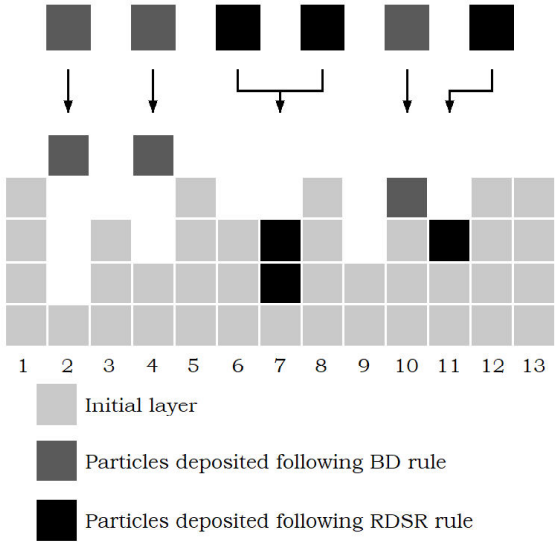

Fig. 1: A pictorial illustration of the deposition scheme in 1+1 dimensions.

Result and Discussion

Fig. 2 shows the variation of ln(W) with respect to ln(t) for the model for system size L = 32 for different values of the competitive growth parameter p.

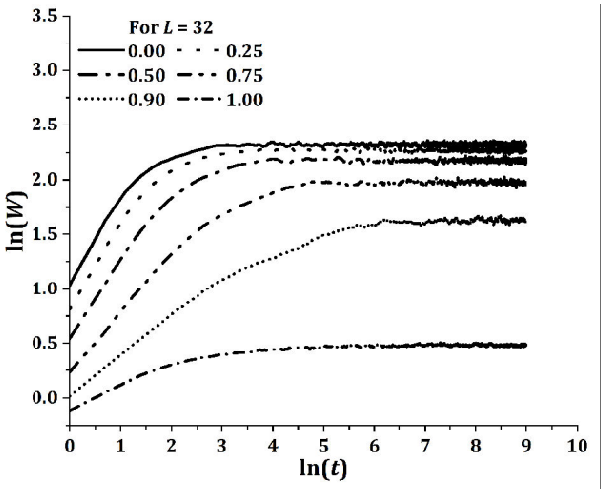

Fig. 2: ln(W) vs. ln(t) graph for L = 32 for different values of p.

Fig. 3 shows the variation of ln (W) with respect to ln(t) for the model for competitive growth parameter p = 0.25 for different values of the system size L.

From Fig. 2 and Fig. 3, it is evident that the first growth exponent β_1 is independent of the system size L but varies with the competitive growth parameter p. In the same manner, the second growth exponent β_2 is also independent of the system size L but varies with the

competitive growth parameter p. From these two figures, it is also evident that the saturation interface width value W_{sat} depends on the system size L and on the competitive growth parameter p. The depicted variations in Fig. 2 and Fig. 3, insinuate the existence of two different critical times. The first critical time t_x separates the first two regimes of time growth, and the second critical time t_{sat} separates the second time growth regime from the saturation regime. The first critical time t_x appears to be independent of the system size L but varies with the competitive growth parameter p. The second critical time t_{sat} appears to be varying with the system size L and with the competitive growth parameter p as well.

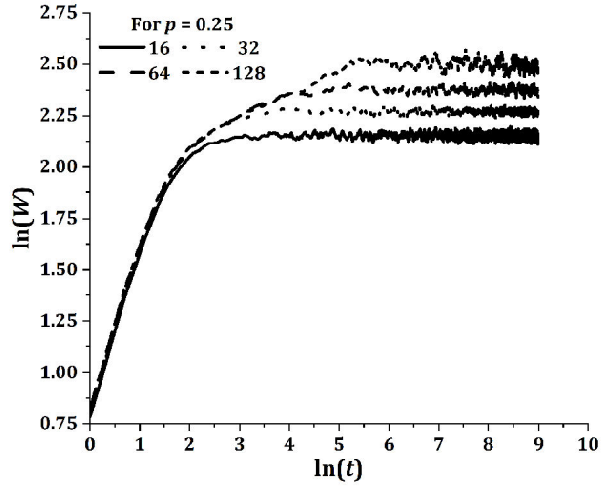

Fig. 3: ln(W) vs. ln(t) graph for p = 0.25 for different values of L.

The variations of these growth exponents with the competitive growth parameter p are shown in Fig. 4. As evident from Fig. 4, the first growth exponent β_1 decreases with the increase in the competitive growth parameter following some power-law relation. The second growth exponent β_2 shows some polynomial (g^{th} order) variation with the competitive growth parameter p as evident in Fig. 4.

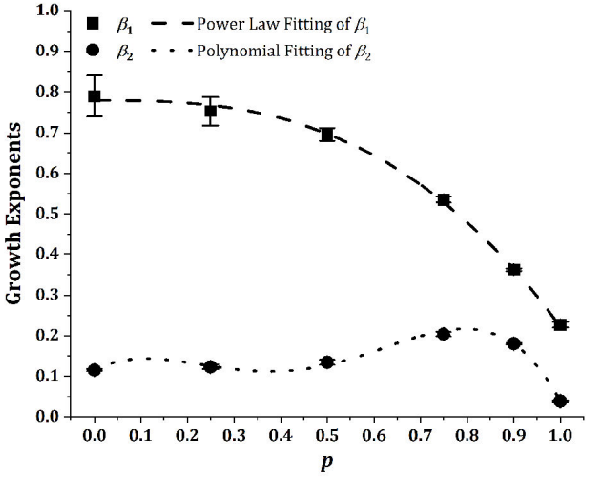

Fig. 4: Growth exponents vs. p graph and relevant fitting curves

Fig. 5 shows the dependence of the saturation interface width value W_{sat} on the competitive growth parameter p.

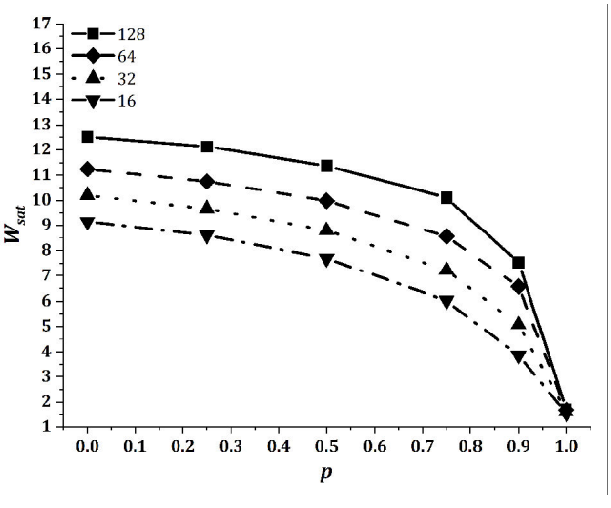

Fig. 5: W_{sat} vs. p graph.

Fig. 6 shows the variation of ln(W_{sat}) with respect to ln(L) for the model for different values of the competitive growth parameter p. The slope of the ln(W_{sat}) vs. ln(L) graph gives the value of the roughness exponent α . Fig.6 confirms that the roughness exponent α varies with the competitive growth parameter p.

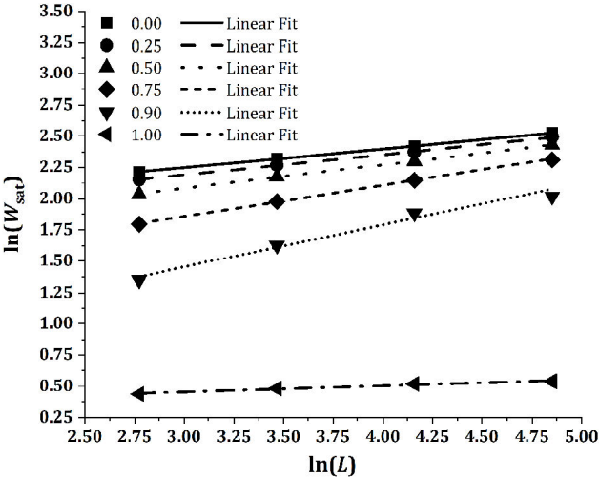

Fig. 6: ln(W_{sat}) vs. ln(L) graph for different values of p and relevant linear fitting curves

The dependence of the roughness exponent α on the competitive growth parameter p is shown in Fig. 7. The roughness exponent α increases exponentially with an increase in the competitive growth parameter p till

p = 0.90 then abruptly drops to a value 0.05. The values of the roughness exponent are completely different from those in Table-1.

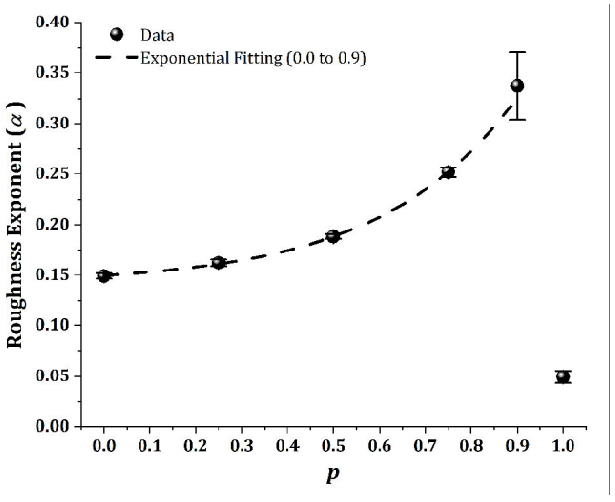

Fig. 7: α vs. p graph for the model and relevant fitting curve

The value of the dynamic exponent z is estimated using the relation $z = \alpha/\beta_2$ which is also independent of the system size L but varies with the competitive growth parameter p. The values of α, β_2, z and $\alpha + z$ for different values of the competitive growth parameter p are shown in Table-2.

Table 2: Values of the scaling exponent α, β_2, z and $\alpha + z$ for different values of the competitive growth parameter p for the model

p	α	β_2	z	$\alpha + z$
0.00	0.15	0.12	1.25	1.40
0.25	0.16	0.12	1.33	1.49
0.50	0.19	0.13	1.46	1.65
0.75	0.25	0.20	1.25	1.50
0.90	0.34	0.18	1.89	2.23
1.00	0.05	0.04	1.25	1.30

The variation of the first critical time t_x with the competitive growth parameter p is shown in Fig. 8. The first critical time t_x increases exponentially with an increase in the competitive growth parameter p till p = 0.90 then abruptly drops to a value close to 8-time units.

The variations of the second critical time t_{sat} with the competitive growth parameter p for different values of system size L are shown in Fig. 9. Similar to the first critical time t_x, the second critical time t_{sat} also increases exponentially with an increase in the competitive growth

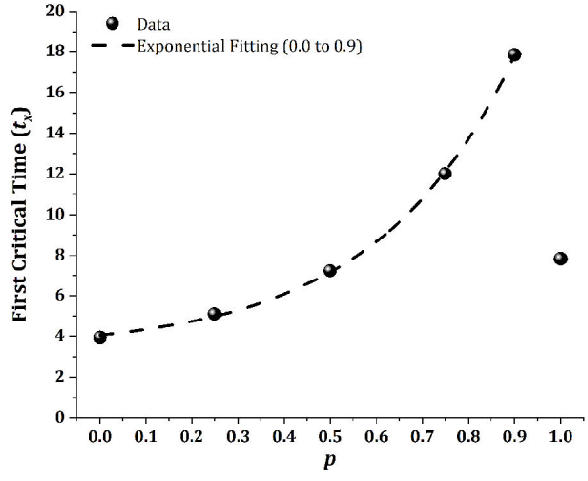

Fig. 8: t_x vs. p graph for the model and relevant fitting curve.

parameter p till p = 0.90 then abruptly drops to a lower value.

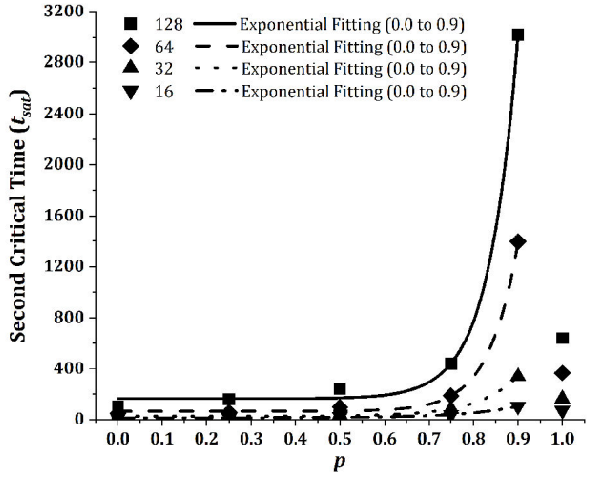

Fig. 9: t_{sat} vs. p graph for different values of L and relevant fitting curves.

The existence of two regimes of time growth and a saturation regime for the model leads to a new scaling approach. The proposed scaling is as follows:

$$\left.\begin{array}{lll} W(t) \sim t^{\beta_1} & \text{for} & t < t_x \\ W(t) \sim t^{\beta_2} & \text{for} & t_x < t < t_{sat} \\ W(L) \sim L^{\alpha} & \text{for} & t < t_{sat} \end{array}\right\} \quad (5)$$

The abrupt decrease in α, z, $\alpha + z$, t_x, and t_{sat} after p = 0.90, indicates a phase transition effect. The tabulated data confirms that the scaling exponent values show deviation from the values mentioned in Table-1 as they vary with the competitive growth parameter p.

The fractional porosity σ of the medium is independent of the system size L but decreases exponentially with an increase in the competitive growth parameter p. The variation is shown in Fig. 10.

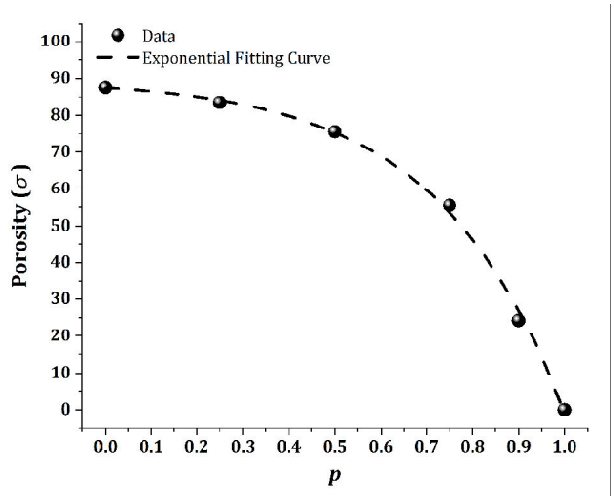

Fig. 10: σ vs. p graph for the model and relevant fitting curve.

Conclusion

For the simulation study of scaling exponents of a rough surface developed for competitive growth between RDSR and BD in 2+1 dimensions. The evolution of the surface roughness appeared with two regimes of time growth with two acutely different slopes and a saturation regime with zero slopes. This requires a new scaling approach, as proposed. The first growth exponent is independent of the system size but has some power-law dependence on the competitive growth parameter. The second growth exponent is independent of the system size but has some polynomial dependence on the competitive growth parameter. The saturation values of the interface width have some reliance on both the system size and the competitive growth parameter. The roughness exponent increases exponentially with an increase in the competitive growth parameter until 0.90 and then abruptly falls to a value of 0.05. The first critical time is independent of the system size but increases exponentially with an increase in the competitive growth parameter until 0.90 and then abruptly falls to a value of 8-time units. The second critical time shows some dependence on the system size and the competitive growth parameter. The second critical time also increases exponentially with an increase in the competitive growth parameter until 0.90 and then abruptly falls to a lower value. The scaling exponents are found to have some deviation from the relevant universality classes and depend on system size and the competitive growth parameter for this model. This kind of abrupt variation in the scaling exponents and critical times has been reported for the first time. The fractional porosity is independent of the system size and decreases exponentially to zero with an increase in the competitive growth parameter.

Acknowledgement

My sincere gratitude is extended in particular to Dr. Jitendra Nath Roy, Professor of Physics, Kazi Nazrul University and Dr. Diptonil Banerjee, Associate Professor of Physics, Teerthankar Mahaveer University for their encouragement, guidance and support. ❐

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