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Comparison of High Field Electron Transport Properties in Wurtzite Phase of ZnO, GaN and SiC

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Abstract: Temperature and doping dependencies of electron drift velocity in wurtzite ZnO structure have been calculated using ensemble Monte Carlo method and compared with electron drift velocity in GaN and SiC in steady-state and transient situation. The following scattering mechanisims i.e., impurity, polar optical phonon and acoustic phonon are inculded in the calculation. The maximum electron drift velocity that is obtained in room temperature for 10^{23} m^{-3} donor concentration are 2.2×10^{7}, 3×10^{7} cm sec^{-1} for ZnO and GaN, respectively. SiC shows the negative differential mobility just in low temperature. For high applied electric field transient electron drift velocity shows a significant overshoot in ZnO and GaN.

Key words: Ensemble Monte Carlo, drift velocity, overshoot, steady-state, scattering mechanisims, temprature

INTRODUCTION

At the start of the 21st century the wide band-gap semiconductors like ZnO, GaN and SiC (with band-gap 3.43, 3.39 and 3.2 eV, respectively) are on the rise and may be regarded as third-generation semiconductors after Si (first-generation with band-gap 1.12 eV) and GaAs and InP (second-generation with band-gap 1.43 and 1.35 eV, respectively). The control of free-carrier concentration is vital for the performance of all semiconductor devices. The intrinsic carrier concentration is exponentially dependent on the temperature:

$$n_i = \sqrt{N_C N_V}\, e^{-E_g/2k_B T}$$

Where:
E_g = The band-gap
k_B = Boltzmann's costant
T = The temperature in Kelvin

It is evident that in high temperatures the wide band-gap semiconductors like ZnO, GaN and SiC have much lower intrinsic carrier concentrations than Si and GaAs. This implies that devices for higher temperatures should be fabricated from wide band-gap semiconductors to avoid the effects of thermally generated carriers (Ashcroft and Mermin, 1975). Also, the wide band-gap semiconductors are of potential interest as a suitable material for high power electronics and because of their direct band gap are benefit for optoelectronic devices too. ZnO has recently received much attention because of its potential advantages over GaN including commercial availability of bulk single crystals, amenability to wet chemical etching and a large exciton binding energy (60 meV compared with 25 meV for GaN) that causes excitonic emission at room and higher temperatures. The exellent radiation hard characteristics make ZnO a suitable candidate for space applications (Albrecht *et al*., 1999; Ozgur *et al*., 2005; Bertazzi *et al*., 2007; Farahmand *et al*., 2001). The present research studies the high-field transport properties for electrons in bulk ZnO and compares its properties with GaN and SiC in both steady-state and transient situations using ensemble Monte Carlo.

MATERIALS AND METHODS

In this research for studying of the electron transport within a semiconductor an ensemble Monte Carlo approach is used in order to solve the Boltzman Transport Equation (BTE), the BTE describes how the electron distribution function evolves under the action of an applied electric field. In this approach the motion of a large number of electrons within a semiconductor, under the action of an applied electric field is simulated.

The acceleration of each electron in the applied electric field and the present of the scattering are both taken into account. The scattering events that an individual electron experiences are selected randomly, the probability of each such event being selected in proportion to the scattering rate corresponding to that particular event. The analysis of electron transport is restricted within the conduction band. Typically, only the lowest part of the conduction band contain a

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Table 1: Important parameters used in the simulations for wurtzite phase ZnO, GaN and SiC (Arabshahi, 2009a, b)

Material parameters	GaN	ZnO	SiC
Mass density (kg m^{-3})	6150.000	5600.000	3200.00
Sound velocity (m sec^{-1})	4330.000	6400.000	1373.00
Static relative permittivity (ε_0)	9.500	8.200	9.70
High frequency relative permittivity (ε_∞)	5.350	3.700	6.50
Acoustic deformation potential (eV)	8.300	14.000	15.00
Polar optical phonon, $h\omega_{op}$ (meV)	99.000	72.000	120.00
Direct energy gap E_g (eV)	3.500	3.430	3.20
Valley parameters	Γ	U	K
Electron effective mass (m^*/m_0)			
GaN	0.200	0.400	0.30
ZnO	0.250	0.400	0.30
SiC	0.280	0.390	0.54
Nonparabolicity coficients (eV^{-1})			
GaN	0.189	0.065	0.70
ZnO	0.312	0.059	0.65
SiC	0.320	0.500	0.03
Valley seperation (eV)			
GaN	0.000	2.000	3.10
ZnO	0.000	2.100	2.90
SiC	0.000	0.610	0.67
Equivalent valley number	1.000	6.000	2.00

significant fraction of the electron population instead of including the entire electron band structure for the conduction band so only the lowest valleys need to be represented and in this study a three valley model is used (O'Leary *et al*., 2006; Jacoboni and Lugli, 1989; Moglestue, 1993).

Within the framework of this three valley model, the nonparabolicity of each valley is treated through the application of the Kane model, the energy band corresponding to each valley being assumed to be spherical and is the form of (Jacoboni and Lugli, 1989; Moglestue, 1993):

$$E(k)[1+\alpha_i E(k)] = \frac{\hbar^2 k^2}{2m^*}$$

where, m^* is the electron effective mass in ith valley and α_i is the nonparabolicity coficient in ith valley.

The scattering mechanisms considered are ionized impurity, polar optical phonon, acoustic diformation potential and intervalley scattering.

For steady-state and transient electron transport simulations the motion of eighty thousand electrons are examined in three valleys of Γ, U and K. The material parameters and valley parameters that are used in this simulation are mentioned in Table 1.

RESULTS AND DISCUSSION

Steady-state electron transport: Figure 1 shows the velocity-field characteristics that obtained by the model for ZnO, GaN and SiC wurtzite in 300 K and with the 10^{23} m^{-3} donor concentration. They have a peak in its velocity field characteristic and so show the negative

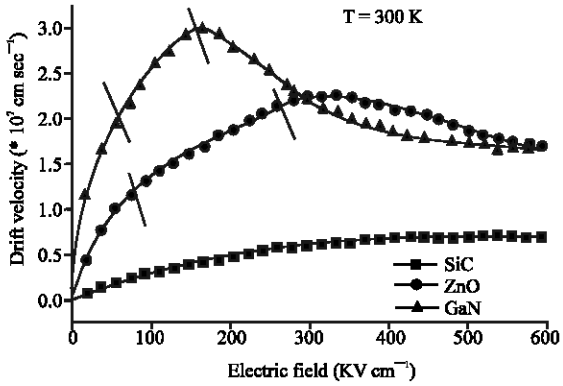

Fig. 1: Calculated electron drift velocity in wurtzite ZnO, GaN and SiC at T = 300 K and 1023 m^{-3} impurity concentration

differential mobility exept for SiC. The peak drift velocity for GaN is around 3×10^7 cm sec^{-1} and for ZnO is about 2.24×10^7 cm^{-1} in threshold fields of 180 kV cm^{-1} and 340 kV cm^{-1}, respectively.

For GaN the peak velocity is larger and occurs at lower electric field thatis because of its lower effective mass in Γ valley. As the effective mass of the electrons in the upper valleys is greater than that in the lowest valley, the electron in the upper valleys will be slower.

As more electrons transfer to the upper valleys the electron drift velocity decreases (Bertazzi *et al*., 2007; O'Leary *et al*., 2006).

This shown the negative differential mobility in Fig. 1 for ZnO and GaN. The other important things that is shown in Fig. 1 is dependence of drift velosity on electric field in ZnO and GaN shown a dual-slope behaviour before the peak velocity which may be traced back to the onset of polar optical scattering (Furno *et al*., 2008).

The valley occupation for the Γ, U and K valleys are shown in Fig. 2. For fields lower than the threshold field, most of the electrons are in the central valley and significant intervalley scattering into the satellite valleys occurs just for fields above the threshold field.

The steady-state electron drift velocity versus electric field has been calculated for these materials at different temperatures and various doping concentrations that are shown in Fig. 3 and 4.

It can be seen in Fig. 3 that the temperatur increasing causes the drift velocity decreasing. Because the temperature increasing increases the acoustic phonon scattering and impurity scattering so the electron mobility and drift velocity decreases (Moglestue, 1993). On the other hand the peak velocity occurs in the higher

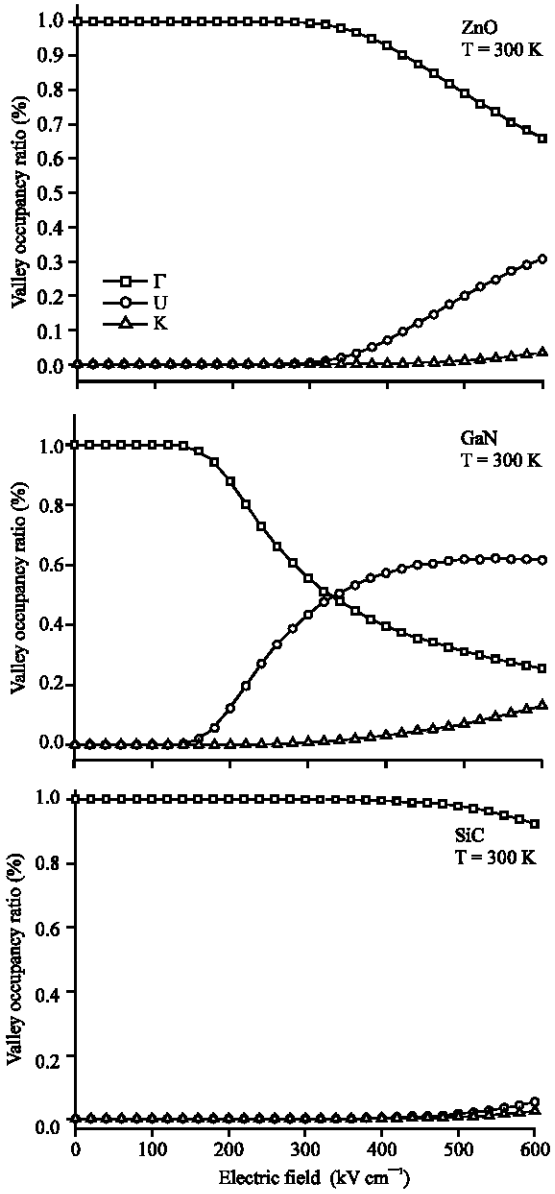

Fig. 2: Calculated valley occupancy ratio in wurtzite ZnO, GaN and SiC at T = 300 K and 10^{23} m^{-3} impurity concentration

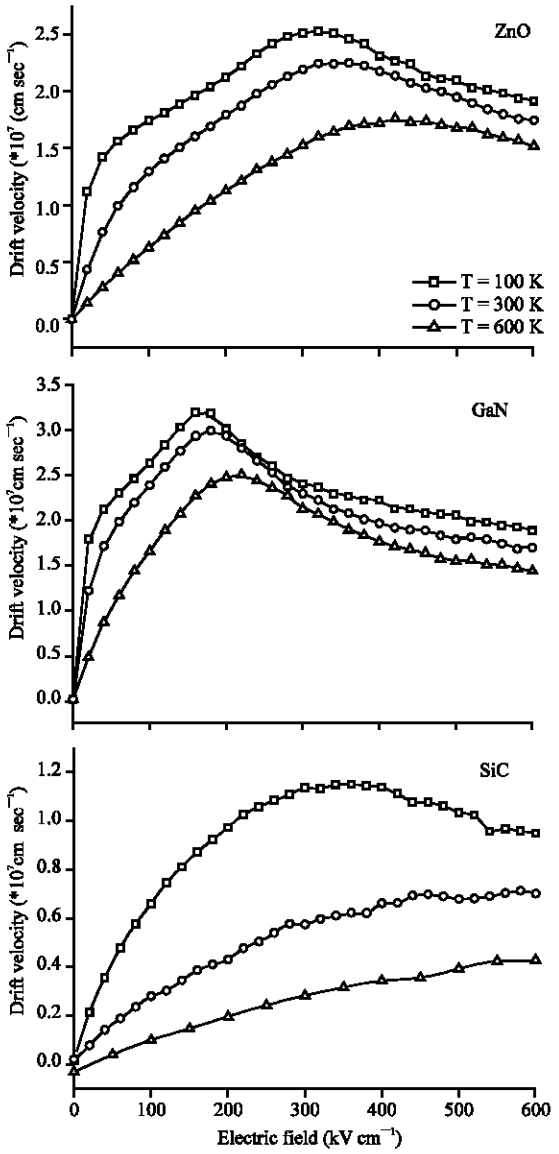

Fig. 3: Calculated electron drift velocity in wurtzite ZnO, GaN and SiC at 10^{23} m^{-3} impurity concentration and different temperatures

electric fields when the temperature increases. It's interesting that for SiC the negative differential mobility is observed in low temperature so it may be seen in higher temperature too but in higher electric fields. Figure 4 shows the various dopping concentration do not have considerable effect on the drift velocity. Because the scattering of ionised impurity is dominated in low temperatures so the drift velocity doesn't affect of changing the dopping concentration in room temperature (Ashcroft and Mermin, 1975).

Transient electron transport: Figure 5 shows the transient behaviour simulated in ZnO, GaN and SiC. In ZnO and GaN for the applied electric field lower than the threshold field electron drift velocity reaches steady-state very quickly with little or no velocity overshoot.

In contrast for applied electric field that are larger than threshold field transient electron drift velocity shows a significant overshoot. In low electric fields the most of electrons are in central valley with lower effective mass so the scattering rate is low and transient drift velocity reaches steady-state quickly. But by increasing the applied electric field electrons can gain more

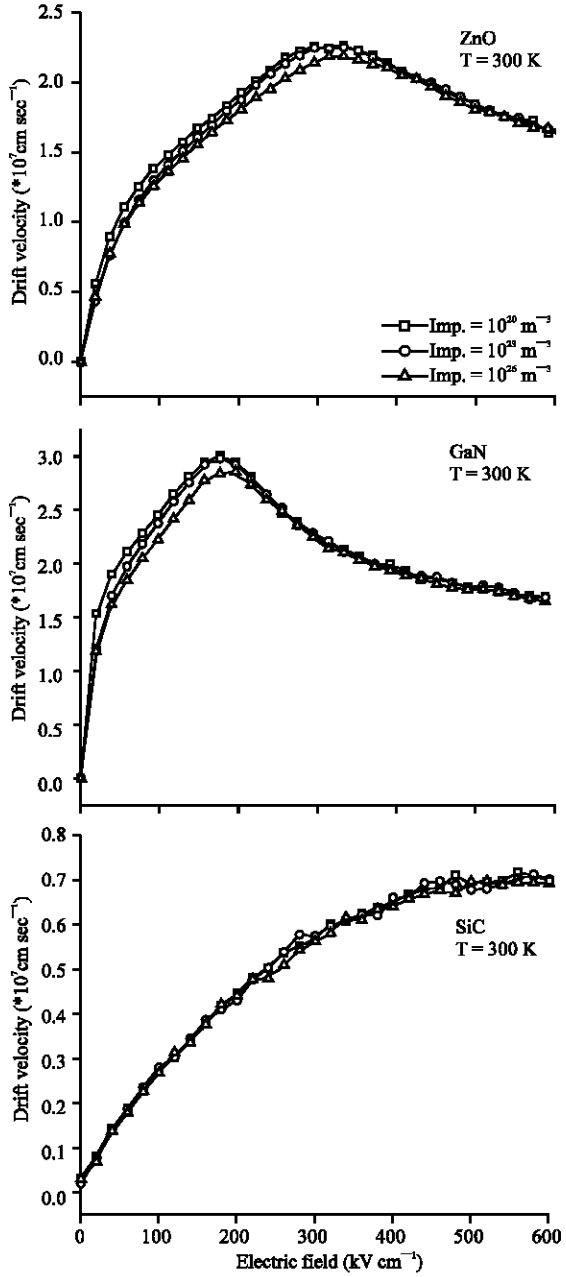

Fig. 4: Calculated electron drift velocity in wurtzite ZnO, GaN and SiC at T = 300 K and different impurity concentrations

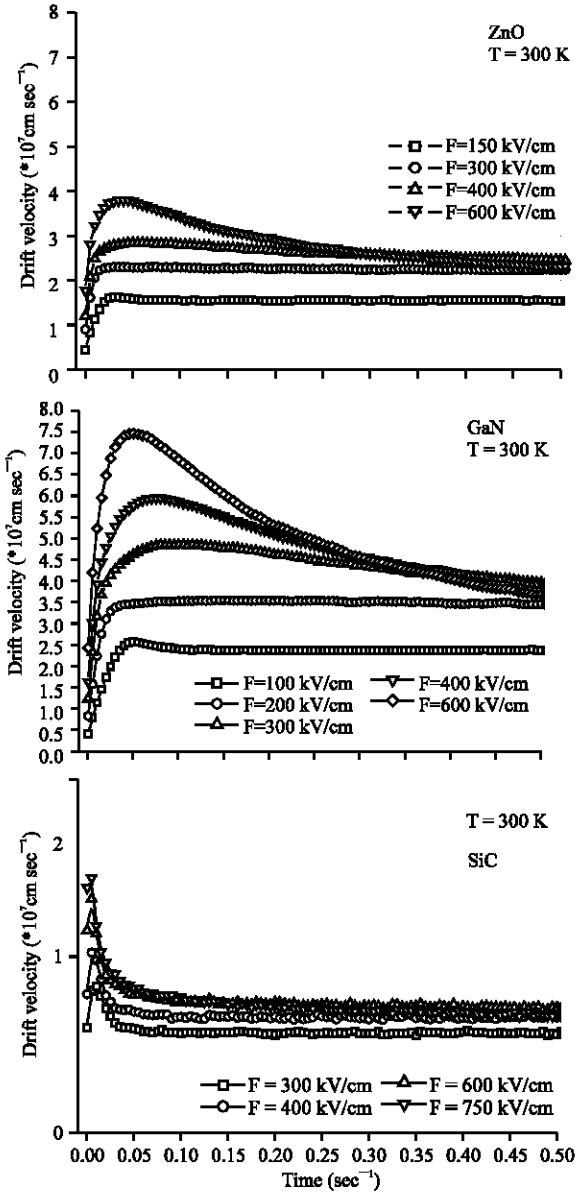

Fig. 5: The calculated time evolution of the electron drift velocity in wurtzite ZnO, GaN and SiC at T = 300 K for different values of the electric field

energy and by pass the time they could go to the upper valley (O'Leary *et al*., 2006). In upper valleys, electron effective mass is larger and it causes the scattering rate increases too. When the scattering rate increases the drift velocity decreases and an overshoot occurs. If applied electric field become more larger because the electron can gain energy of field sooner the overshoot occures sooner too. In SiC because the valley seperations are lower than ZnO and GaN, the overshoot occures very soon. But because the electron effective mass in its Γ valley are larger than ZnO and GaN, the drift velocity peak magnitude is lower.

Transient behaviour depependence on temperature are shown in Fig. 6 for two applied electric field one of them is lower than threshold field and another is larger than threshold field. It can be seen for constant electric field when temperature increases like the

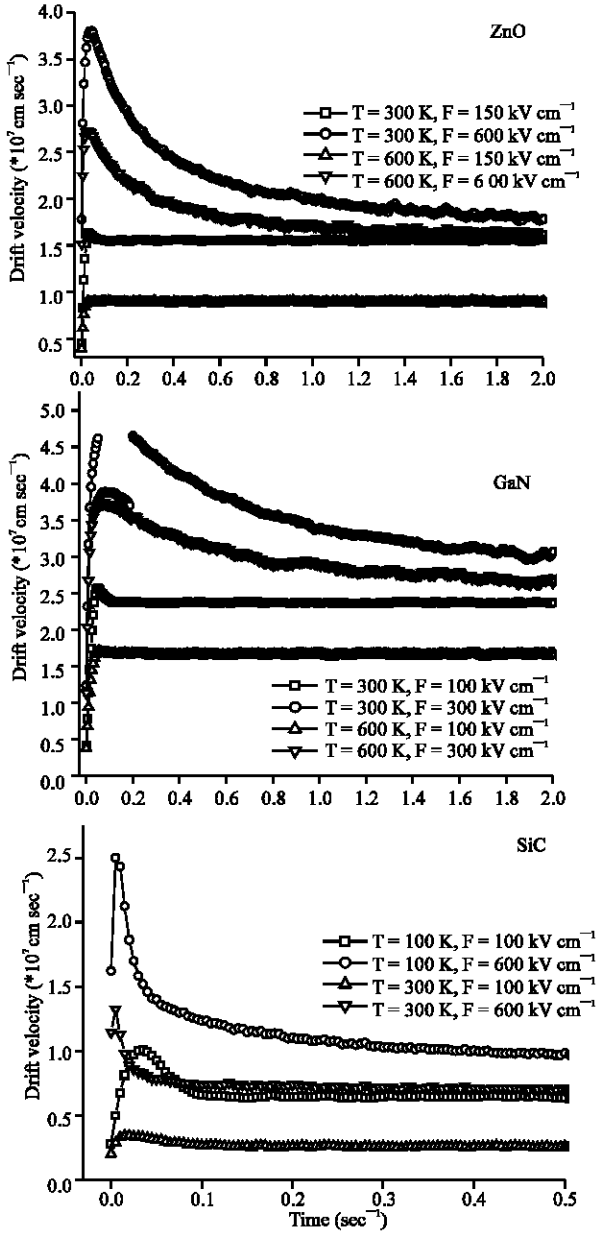

Fig. 6: The calculated time evolution of the electron drift velocity in wurtzite ZnO, GaN and SiC for different values of the electric fields and temperature

steady-state situation because of increasing scattering rate drift velocity decreases but the time behaviour is independent of temperature. Transient drift velocity versus distance is also calculated. The result is shown in Fig. 7. Like the transient drift velosity versus time, it can be seen in SiC drift velocity reaches the steady-state sooner than ZnO and GaN. Also, in applied electric field larger than threshold field because of increasing scattering rate, drift velocity reaches to steady-state in longer distance.

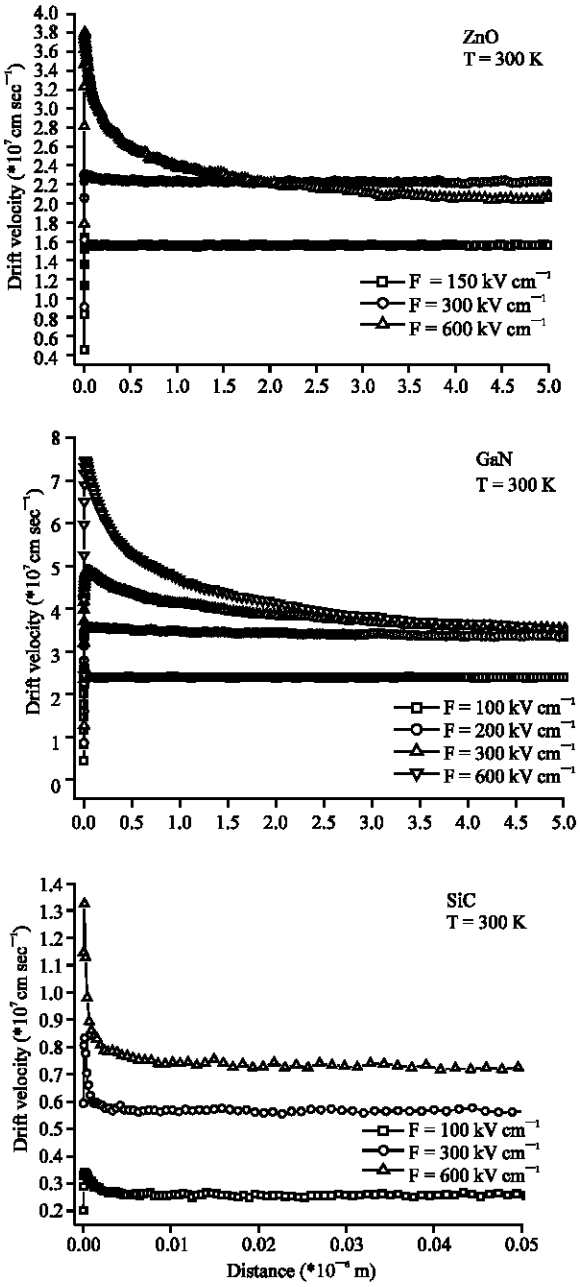

Fig. 7: The calculated distance evolution of the electron drift velocity in wurtzite ZnO, GaN and SiC at T = 300 K for different values of the electric fields

CONCLUSION

This research presents a steady-state and transient transport study of wurtzite ZnO, performed with ensemble Monte Carlo simulation and compare results with GaN and SiC.

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